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Evaluation of Military Field-Water Quality
Volume 2. Constituents of Military Concern from
Natural and Anthropogenic Sources
Part 1. Organic Chemical Contaminants

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January 1988

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However, we identified several organic solutes that could cause taste and odor problems. These compounds include trichloromethane, ethylbenzene, toluene, tetrachloroethene, and chlorinated phenols. Additionally, geosmin and 2-methylisoborneol, which are two metabolites of blue-green algae (*cyanobacteria*) and associated gram-negative filamentous bacteria (*actinomycetes*), can produce taste and odor problems and are of particular concern, especially when algal blooms are present. Oil and grease could also impair the potability of water supplies, and by fouling reverse-osmosis (RO) membranes, oil and grease could impair the performance of reverse osmosis water purification units (ROWPUs).

This report is the first part of the second volume of a nine-volume study entitled Evaluation of Military Field-Water Quality. The second and third parts of this volume address pesticides and inorganic chemicals, respectively. Titles of the other volumes are as follows: Vol. 1, Executive Summary; Vol. 3, Opportunity Poisons; Vol. 4, Health Criteria and Recommendations for Standards; Vol. 5, Infectious Organisms of Military Concern Associated with Consumption: Assessment of Health Risks, and Recommendations for Establishing Related Standards; Vol. 6, Infectious Organisms of Military Concern Associated with Nonconsumptive Exposure: Assessment of Health Risks, and Recommendations for Establishing Related Standards; Vol. 7, Performance Evaluation of the 600-GPH Reverse Osmosis Water Purification Unit (ROWPU): Reverse Osmosis (RO) Components; Vol. 8, Performance of Mobile Water Purification Unit (MWP) and Pretreatment Components of the 600-GPH Reverse Osmosis Water Purification Unit (ROWPU) and Consideration of Reverse Osmosis (RO) Bypass, Potable-Water Disinfection, and Water-Quality Analysis Techniques; and Vol. 9, Data for Assessing Health Risks in Potential Theaters of Operation for U.S. Military Forces.

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Evaluation of Military Field-Water Quality

Volume 2. Constituents of Military Concern from Natural and Anthropogenic Sources

Part 1. Organic Chemical Contaminants

D. W. Layton, B. J. Mallon, T. E. McKone,
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FOREWORD

This report is the first part of the second volume of a nine-volume study entitled Evaluation of Military Field-Water Quality. The second and third parts of this volume address pesticides and inorganic chemicals, respectively. Titles of the other volumes are as follows: Vol. 1, Executive Summary; Vol. 3, Opportunity Poisons; Vol. 4, Health Criteria and Recommendations for Standards; Vol. 5, Infectious Organisms of Military Concern Associated with Consumption: Assessment of Health Risks, and Recommendations for Establishing Related Standards; Vol. 6, Infectious Organisms of Military Concern Associated with Nonconsumptive Exposure: Assessment of Health Risks, and Recommendations for Establishing Related Standards; Vol. 7, Performance Evaluation of the 600-GPH Reverse Osmosis Water Purification Unit (ROWPU): Reverse Osmosis (RO) Components; Vol. 8, Performance of Mobile Water Purification Unit (MWPU) and Pretreatment Components of the 600-GPH Reverse Osmosis Water Purification Unit (ROWPU) and Consideration of Reverse Osmosis (RO) Bypass, Potable-Water Disinfection, and Water-Quality Analysis Techniques; and Vol. 9, Data for Assessing Health Risks in Potential Theaters of Operation for U.S. Military Forces.

As indicated by the titles listed above, the nine volumes of this study contain a comprehensive assessment of the chemical, radiological, and biological constituents of field-water supplies that could pose health risks to military personnel as well as a detailed evaluation of the field-water-treatment capability of the U.S. Armed Forces. The scientific expertise for performing the analyses in this study came from the University of California Lawrence Livermore National Laboratory (LLNL) in Livermore, CA; the University of California campuses located in Berkeley (UCB) and Davis (UCD), CA; the University of Illinois campus in Champaign-Urbana, IL; and the consulting firms of IWG Corporation in San Diego, CA, and V.J. Ciccone & Associates (VJCA), Inc., in Woodbridge, VA. Additionally a Department of Defense (DoD) Multiservice Steering Group (MSG), consisting of both military and civilian representatives from the Armed Forces of the United States (Army, Navy, Air Force, and Marines), as well as representatives from the U.S. Department of Defense, and the U.S. Environmental Protection Agency provided guidance, and critical reviews to the researchers. The reports addressing chemical, radiological, and biological constituents of field-water supplies were also reviewed by scientists at Oak Ridge National Laboratory in Oak Ridge, TN, at the request of the U.S. Army. Furthermore, personnel at several research laboratories, military installations, and agencies of the U.S. Army and the other Armed Forces provided technical assistance and information to the researchers on topics related to field water and the U.S. military community.

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**EVALUATION OF MILITARY FIELD-WATER QUALITY
VOLUME 2. CONSTITUENTS OF MILITARY CONCERN FROM
NATURAL AND ANTHROPOGENIC SOURCES**

Part 1. Organic Chemical Contaminants

PREFACE

Water that may be used by military personnel in the field can contain many different organic and inorganic chemical constituents. These chemicals may exist in a dissolved or colloidal state or on suspended material, and they are present as a consequence of either natural geochemical and hydrological processes or the industrial, domestic, or agricultural activities of man.

The health risk to military personnel from a chemical constituent of field water is largely a function of the frequency with which it occurs at concentrations that are high enough to produce a toxic or organoleptic (e.g., detectable taste or odor) effect that leads directly or indirectly to the diminished ability of exposed military forces to perform assigned tasks. To minimize performance-related effects in military personnel using field-water supplies, the high-risk chemical constituents must be identified and analyzed. The potential health risks of the contaminants can then be managed by adopting and meeting field-water quality standards. The health effects that could occur when standards are exceeded can be addressed on a case-by-case basis.

The objective of Volume 2 of Evaluation of Military Field-Water Quality is to indicate the chemical constituents of field water that are of possible military concern and to describe the screening methodology and supporting data that we used to identify them. Briefly, the screening methodology is separated into two phases. In both phases the general approach consists of comparing (1) the maximum likely concentration in field water of each possible chemical constituent with (2) a corresponding concentration we estimate to be the threshold above which toxic effects, including impaired performance, could occur. Our analyses are based on 70-kg military personnel consuming field water at a maximum rate of 15 L/d. Maximum likely concentrations in field water for each chemical are derived from our compilation of available U.S. and worldwide water-quality monitoring data. However, in the first phase of screening we make conservative assumptions to extrapolate the threshold concentration above which toxic effects could occur in military forces from either oral-mammalian LD₅₀ (lethal dose to 50% of a population) data or Acceptable Daily Intake (ADI) values for humans. The result of this screening procedure is to exclude from further consideration those chemical constituents

that are not expected to be of military concern. Although the conservative assumptions incorporated into the initial screening exercise minimize the omission of substances that may actually be of concern, some substances may be identified incorrectly as high-risk. Therefore, to refine the results of the initial screening effort, we reexamine the available monitoring data and review the published human-toxicity data more carefully for each chemical indicated to be of possible military concern. Next, we use any more appropriate human-toxicity data (e.g., dose-response information from reported accidental poisonings, occupational exposures, or therapeutic administrations) that we find and apply it in the second phase of screening. Then, as in the initial screening procedure, any ratio greater than unity between the maximum likely concentration for a chemical in field water and the concentration above which it could produce toxic or organoleptic effects in 70-kg military personnel consuming field water at a maximum rate of 15 L/d indicates that the chemical really could be of military concern. Because impaired performance can occur as a result of indirect health effects, especially from heat illnesses caused by dehydration resulting from reduced consumption of poor-tasting water, we also screen the initial list of chemicals by comparing maximum likely concentration data for each one with available data corresponding to the concentration of the substance that represents the taste- or odor-detection threshold in water.

To facilitate data acquisition, analysis, and review, as well as application of the screening methodology, we separated the potential chemical constituents of field water into three categories and divided Volume 2 into three corresponding parts. Part 1 covers organic solutes (except pesticides), Part 2 addresses pesticides, and Part 3 focuses on inorganic chemicals.

ABSTRACT

In this part of Volume 2 we focus on the identification and analysis of organic water contaminants that could degrade the performance of military personnel that drink field water. To identify the contaminants of concern, we developed a screening methodology for comparing measured concentrations of organic solutes in U.S. and foreign surface and ground waters against estimated threshold concentrations for toxic and organoleptic effects. If the measured concentration of a substance in water was higher than the concentration used as an effects threshold for toxic or organoleptic responses, we then closely examined the substance's occurrence and toxicity to decide on recommending development of a water standard to protect military personnel from adverse health effects. After comparing the measured concentrations with the threshold concentrations for toxic or organoleptic effects, we concluded that there was only a small probability that troops would experience performance-degrading effects as a result of drinking field water containing organic solutes. However, we identified several organic solutes that could cause taste and odor problems. These compounds include trichloromethane, ethylbenzene, toluene, tetrachloroethene, and chlorinated phenols. Additionally, geosmin and 2-methylisoborneol, which are two metabolites of blue-green algae (cyanobacteria) and associated gram-negative filamentous bacteria (actinomycetes), can produce taste and odor problems and are of particular concern, especially when algal blooms are present. Oil and grease could also impair the potability of water supplies, and by fouling reverse-osmosis (RO) membranes, oil and grease could impair the performance of reverse osmosis water purification units (ROWPUs).

INTRODUCTION

The objective of Volume 2 of Evaluation of Military Field-Water Quality is to identify those water contaminants that have potential for impairing troop performance. Key considerations in identifying hazardous contaminants are their occurrence in foreign water supplies, the concentrations measured, and importantly, their toxicity. Volume 2 is divided into three parts: Part 1 covers organic solutes (except pesticides); Part 2 deals exclusively with pesticides; and Part 3 addresses inorganic solutes.

Of particular concern are health effects that would directly affect an individual's ability to conduct a military mission. Indirect effects, such as heat illnesses caused by dehydration resulting from the reduced consumption of poor-tasting water, are also important. The health risk of an organic contaminant in drinking water is a function of its occurrence, expected concentrations, toxicity, and organoleptic properties. As an illustration, a substance that is toxic at low concentrations in water but is found rarely in surface and ground waters would not be considered a high-risk substance. Accordingly, a basic requirement of a screening methodology for field-water contaminants is that it include those factors that directly influence risk. For example, this methodology must consider occurrence in different water sources, measured or predicted concentrations in water, and finally, concentrations that could cause adverse health responses. Another requirement is that the screening procedure should minimize omission of organic solutes that are actually of concern. This means that the methodology should be based on conservative assumptions, even if some substances are incorrectly identified as high-risk during the initial phases of screening. In the following sections we review the basic methodology for screening organic solutes, the data and procedures used to represent contaminant concentrations, and the data and procedures used to estimate threshold-effect concentrations.

OVERVIEW OF THE SCREENING METHODOLOGY

The basic procedure for screening an organic solute, as shown schematically in Fig. 1, is to compare its measured or predicted concentration in water with a screening concentration which represents a no-effect level; that is, the screening concentration has a low probability of degrading performance or causing an organoleptic response. Figure 2 depicts the various comparisons that can result. If the solute concentration is below the screening concentration for toxic effects and the organoleptic concentration (comparison A), then the substance does not constitute a potential health risk. However, if the concentration is above either of these screening concentrations (i.e., comparisons B to E),

then the substance is considered a potential high-risk contaminant. The highest potential health risk occurs when the odor or taste threshold is above the no-effect threshold, because there is no organoleptic warning of possible danger (comparison E). The second phase of the screening methodology is a more detailed analysis of the toxicity and occurrence of these high-risk solutes to ensure that they are identified correctly.

The presence of organic solutes in natural waters is a complex function of usage, pollution controls, environmental chemistry (e.g., solubility, volatility, decomposition rates, etc.), and transport (i.e., dilution and diffusion) in surface and ground waters. Measured concentrations of a solute reflect all of the above factors. If we knew all of the relevant parameters for different organic compounds, as well as site-specific hydrologic characteristics, we could conceivably predict concentrations in various water supplies. Unfortunately these data are incomplete for most chemicals. Therefore, in order to estimate the probable occurrence of organic chemicals in field-water supplies, we have relied principally on measured concentrations in treated and untreated waters in foreign countries and the U.S. To augment the measured concentration values, we have used a methodology to predict levels of organic contaminants in the surface waters of foreign countries receiving industrial waste waters.

One of the more difficult components of the screening methodology is the calculation of threshold solute concentrations, above which there would be a high probability of toxic effects in humans. Acquisition and analysis of toxicological data on each substance to define these thresholds is an expensive proposition. An alternative is to estimate the thresholds from the more widely available data on mammalian species. The most frequently reported parameter in this regard is the lethal dose (expressed in mg of chemical per kg of body weight) to 50% of a population of laboratory animals (i.e., an LD₅₀). To estimate human threshold concentrations from mammalian data, we use the LD₅₀ of the species most sensitive to the substance of concern. This value is multiplied by a fraction derived from a statistical analysis of the ratios of no-effect dose rates [in mg/(kg•d)] to LD₅₀'s for a set of chemicals. After the applicable dose is calculated, an equivalent concentration in water is calculated, based on a 70-kg man consuming 15 L of water per day. The calculated threshold concentrations are then compared with observed or predicted concentrations in water (see Fig. 1). Those substances that meet the high-risk screening criteria are then scrutinized further to determine whether they are indeed compounds that pose adverse health risks to soldiers that drink field water.

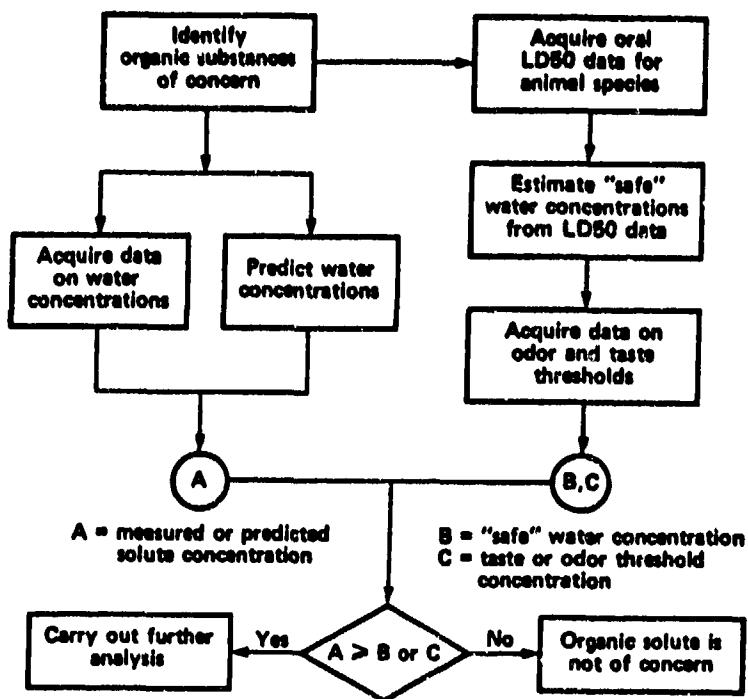


Figure 1. Diagram of the methodology for identifying organic solutes that could pose health risks to military personnel consuming field waters. The basic procedure for screening a chemical is to compare measured or predicted concentrations in water with concentrations that represent a no-effect level. Solutes whose concentrations in water are above toxic or organoleptic thresholds are potentially high-risk compounds.

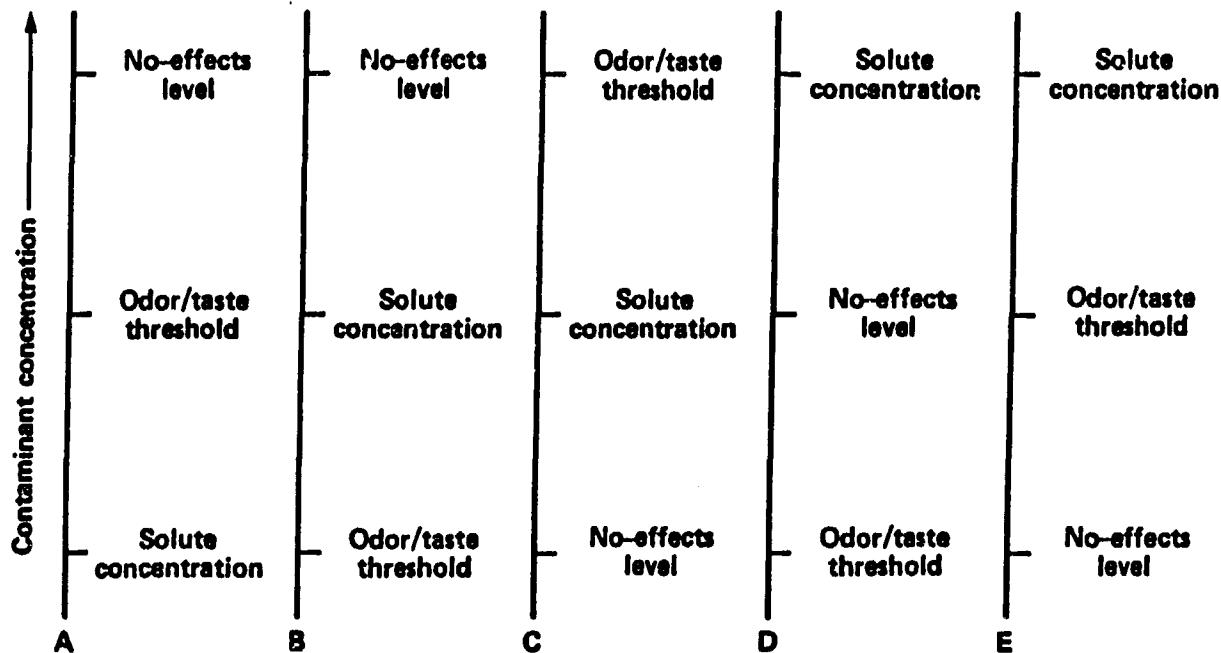


Figure 2. Possible comparisons between water concentrations and threshold concentrations for toxic and organoleptic responses.

IDENTIFICATION OF ORGANIC CONTAMINANTS

It would be impossible to complete screening analyses on all organic compounds that are potential water contaminants. Accordingly, the goal of our data-gathering efforts was to focus on those substances that might actually constitute a health threat to troops drinking treated or untreated field water. The substances identified for screening analyses included organic substances for which health standards had been established by domestic or foreign governments or scientific organizations and substances that appeared on hazardous material lists. Our premise was that such standards and lists reflect objective and subjective evaluations of the health risks of various organic solutes in water supplies worldwide. We supplemented this set of compounds with substances that were reported in foreign water supplies and substances that were measured frequently in U.S. water supplies. The primary emphasis, though, was on measured concentrations of organic solutes in foreign water resources because these supplies are the most likely sources of field drinking waters. The final screening list consisted of over 200 potentially hazardous substances (see Appendix A).

SCREENING CONCENTRATIONS FOR TOXIC AND ORGANOLEPTIC RESPONSES

In this section we describe the methodology we used to derive the minimum concentrations of organic solutes in field water that could produce toxic effects in military personnel consuming up to 15 L of water per day. These minimum concentrations represent the screening concentrations for toxic effects. We also discuss the data used to identify contaminants that could cause organoleptic responses in exposed individuals.

TOXIC EFFECTS

A major challenge in developing a methodology for identifying organic solutes that could pose adverse health risks to soldiers is the quantification of a screening concentration for toxic effects. Ideally, we would calculate the equivalent screening concentration for toxicity as follows:

$$C_s = \frac{NOEL}{SF} \cdot \frac{W}{I}, \text{ where} \quad (1)$$

C_s = screening concentration for human toxicity, mg/L;

NOEL = maximum no-observed-effect level in rats, mg/(kg·d);

- SF - safety factor for adjusting the animal data to compensate for intra- and interspecies variation, dimensionless;
- W - reference body weight of a soldier, kg; and
- I - maximum daily intake of water, L/d.

Unfortunately, the no-observed-effect levels (NOEL's) derived from animal studies are available for only a relatively small number of substances. The data that best meet the criteria for availability are the oral LD50 data for mammalian species. The LD50, however, is not particularly useful for developing a screening dose or concentration because there is no direct way to relate this acute measure of animal toxicity (i.e., lethality) to an effects threshold in humans. To relate LD50 data to screening concentration thresholds, we adopted a statistical approach in which an LD50 is used to define a lower-bound limit of toxic effects, based on a statistical analysis of the relationship between LD50 values and subchronic (90-d) NOEL's. McNamara,¹ in a study of the relationship between chronic and acute toxicities, computed the ratios of subchronic NOEL's [mg/(kg•d)] to LD50's (oral administrations to rats, mg/kg) for 33 substances. The geometric mean of the log normally distributed ratios was 0.03 d^{-1} with a geometric standard deviation of 4.8. A conservative NOEL (i.e., a NOEL that has a high probability of being below a toxic threshold) can then be calculated from an LD50 by multiplying the median lethal dose by a ratio that corresponds to a suitable cumulative percentile on the lognormal distribution. For the purposes of this screening exercise, we chose the ratio corresponding to the 10th cumulative percentile of the lognormal distribution, or 0.004 d^{-1} (i.e., $0.03/4.8^{1.3}$).

The 90-d exposure period used for the NOEL is similar to a human exposure period of nearly ten years, based on the assumption that the ratios of the two periods to the lifespans of the respective species are approximately the same (i.e., 90 d/730 d = 9 y/75 y). By comparison, the assumed exposure period for consuming field-water supplies is one year, and so there is an implicit margin of safety in using the derived subchronic NOEL. A safety factor of 100 was selected to adjust the NOEL because this factor has been widely used by regulators for standards setting, and it is supported by data on inter- and intraspecies variations (see Dourson and Stara²). The reference body weight of a soldier is 70 kg, and the maximum intake of drinking water is 15 L/d. In addition, we assume that the military population is predominately male; age ranges from 18 to 50 y; and the troops are in good health. We use these assumptions to calculate the screening concentration, in mg/L, from an animal LD50 (mg/kg) as:

$$C_s = \frac{\text{LD50} \cdot 0.004}{100} \cdot \frac{70}{15} . \quad (2)$$

To simplify the computation of the screening concentrations, we multiplied the LD₅₀ values by 10⁻⁴ to obtain a C_s value. In addition, we used the oral LD₅₀ value of the most sensitive mammalian species; most of these LD₅₀'s were for rats. When oral LD₅₀'s (or intraperitoneal LD₅₀'s in some instances) were not listed in the Registry of Toxic Effects of Chemical Substances,³ we used the lowest lethal doses for oral administrations. Appendix B contains the animal LD₅₀ data used to calculate screening concentrations.

ORGANOLEPTIC RESPONSES

Organic substances dissolved in water can impart undesirable tastes and odors. However, data on the organoleptic properties of organic solutes rarely deal with the objectionability of the tastes and odors. Instead, data are presented on the concentrations at which the odor or taste of a chemical is detected by an individual or panel of testers. Threshold concentrations are reported as individual values, ranges, means, medians, or minima, making it almost impossible to accurately compare the organoleptic properties of chemicals. Moreover, because researchers have not used the same techniques to measure organoleptic responses, the resulting odor and taste thresholds can show large variability -- even for the same compound.⁴ With these difficulties in mind, our approach is to screen the organic chemicals that are potential contaminants of field water, based on their organoleptic properties, by comparing the lowest odor or taste threshold recorded in the literature with the measured or predicted solute concentrations for the chemicals in natural waters (see Appendix C for a listing of the organoleptic data). Substances whose concentration in water is above the measured odor or taste threshold are identified as potential high-risk compounds from an aesthetic standpoint. Once identified, these compounds must be analyzed further to determine whether their tastes or odors are likely to cause adverse responses. In such cases we reviewed the applicable literature on the particular compound.

SCREENING BASED ON MEASURED AND PREDICTED CONCENTRATIONS OF ORGANIC SOLUTES

The screening methodology employs a comparison between our estimated toxic/organoleptic concentration and predicted and measured concentrations of organic substances in water resources located in various parts of the world. Most of our effort was directed toward the acquisition of data on organic solutes in foreign water supplies. Unfortunately, such data were difficult to locate and obtain. One reason for the absence

of data on organic solutes is the lack of the appropriate analytical equipment and water-sampling programs in developing countries, and even industrialized ones. Because of this, we were forced to supplement the foreign data with U.S. data. Whether U.S. data are reasonable surrogates for foreign water supplies is debatable. Nevertheless, the large number of organic substances entering U.S. surface and ground waters from industrial and domestic sources would seem to bracket the kinds of compounds that might be encountered elsewhere; however, less-developed countries are likely to have different industrial mixes (and therefore different waste effluents) and less stringent water pollution controls, which would result in higher solute concentrations. To ensure that the monitoring data we were able to obtain provided a reasonable picture of water contamination expected in foreign water supplies, we also calculated concentrations of organic solutes in surface waters of five countries that receive waste waters from a mix of different industries.

MEASURED SOLUTE CONCENTRATIONS

In order to characterize the concentrations of organic solutes that are apt to occur in foreign field-water supplies, we collected concentration data for many different countries. Table 1 summarizes the measured concentrations for 150 organic substances in major geographic regions of the world. Most of our efforts were directed toward the acquisition of water-quality data for water supplies outside of North America, but we have also included a significant number of samples from the U.S. and Canada to supplement the foreign data. We encoded the appropriate water-quality data for entry into our computerized data base. After the entries were made, we checked the values in the data base against the original values in the source documents. We also analyzed the concentration data statistically to identify unusually high or unusually low values. Whenever such concentrations were identified, we examined the source document to determine their validity. If the validity of the reported concentrations could not be established, we removed the values from the data base. Appendix D contains the concentration data that we were able to obtain from the open literature. Figure 3 is a log probability plot of the maximum concentrations for each of the solutes measured in different studies. This plot clearly shows that nearly all organic solute concentrations are below 1 mg/L.

Table 1. Summary of the organic solute concentration measurements for 150 organic substances in water supplies located in major geographic regions around the world.

Geographic location	Number of concentration values selected for screening
pe	364
North America	235
Southeast Asia	96
Africa	77
Middle East	35
Asia	34
South America	20
Central America	8
Total	869

Screening for Systemic Toxicants

The objective of the first phase of the screening analysis was to identify compounds that could pose health risks by virtue of their frequency of occurrence, measured concentrations, and toxicity. In Table 2 we present the ratios of the maximum measured concentration of each organic solute to the screening concentration we estimated as the threshold for toxicity. The compounds of greatest concern are those with ratios greater than unity (to be conservative, we also examined substances with ratios greater than 0.1). To ensure that the maximum concentration values for compounds with a screening ratio greater than 1 were valid, we compared these values with those independently recorded for the same chemicals in a separate data base named WaterDROP. This data base was prepared under the sponsorship of the U.S. Environmental Protection Agency (EPA). It contains data on over 20,000 occurrences of nearly 1000 organic solutes in different kinds of waters (e.g., industrial effluents, process streams, surface and ground waters, etc.).⁵ We used WaterDROP only as an auxiliary check of our concentration data because we were unable to verify the accuracy of the reported data as waterDROP is no longer supported as a sponsored project of EPA. In Table 3 we show those compounds that had maximum concentrations in WaterDROP greater than the ones we reported and also those compounds with values less than our maximum values.

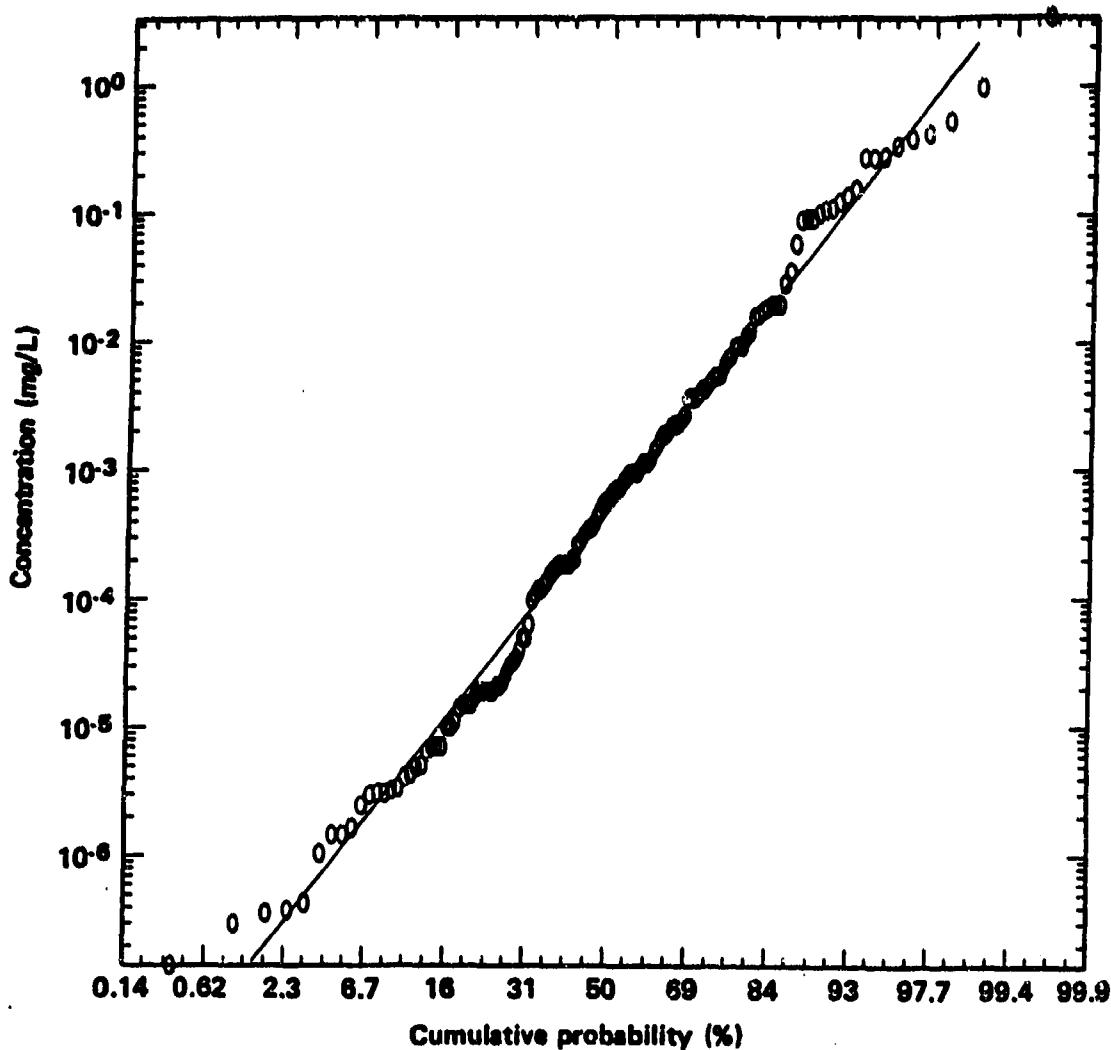


Figure 3. Log probability plot of the maximum concentration for each organic solute that was reported in one or more studies. The geometric mean concentration was 0.0005 mg/L, with a geometric standard deviation of 40. The total number of data points (n) equals 150.

The high concentrations of compounds in surface waters reported in WaterDROP were all in conjunction with immediate (e.g., adjacent to discharge points) industrial pollution. For example, phenol and xylene were both found in surface waters directly receiving effluent from a petrochemical plant. Dilution would diminish these concentrations.

The compound with the highest ratio is trisodium nitrilotriacetate (NTA). Data on the concentrations of NTA were obtained from a study by Woodiwiss *et al.*,⁶ who sampled several Canadian streams receiving sewage effluents from cities in the province of Ontario. The NTA was present in detergents as a replacement for phosphates. The

Table 2. Ratios of maximum observed concentrations (C_{max}) to screening concentrations (C_s) calculated from oral LD₅₀'s for mammalian animal species. The reference code is an abbreviation for the reference containing the concentration data (see Appendix D).

Substance	Water type ^a	C_{max} (mg/L)	C_s ^b (mg/L)	Ratio C_{max}/C_s	Ref.
Phenol, m-chloro-	SW	6.00E-03	5.70E-02	1.05E-01	WEGM79
Phthalate, butylbenzyl	GW	3.80E-02	3.16E-01 ^c	1.20E-01	EPA811
Phenol, 4-chloro-	SW	3.90E-03	2.61E-02	1.49E-01	WEGM79
Aniline, 2-chloro-	SW	3.90E-03	2.56E-02	1.52E-01	WEGM81
Ethane, trichlorotrifluoro-	GW	1.35E-01	8.60E-01 ^c	1.57E-01	EPA811
Ethene, chloro- (vinyl chloride)	FDW	8.40E-03	5.00E-02	1.68E-01	WEST84
Ether, bis(2-chloroisopropyl)	SW	4.60E-03	2.40E-02	1.92E-01	MEIJ76
Benzene, 1,2-dichloro-	SW	1.00E-02	5.00E-02	2.00E-01	PIET80
Ethane, 1,2-dichloro-	FDW	9.80E-03	4.89E-02	2.00E-01	WEST84
Propane, 1,2-dichloro-	FDW	2.10E-02	8.60E-02	2.44E-01	WEST84
Cyclopentadiene, hexachloro-	SW	2.90E-03	1.13E-02	2.57E-01	COTR83
Benzene	GW	1.00E-01	3.80E-01	2.63E-01	DUIJ81
Benzene, 1,4-dichloro-	GW	1.76E-02	5.00E-02	3.52E-01	PAGE82
Phthalate, di-n-butyl	GW	4.70E-01	1.20E+00	3.92E-01	EPA81
Ethene, tetrachloro-	GW	3.75E-01	8.10E-01	4.63E-01	EPA81
Toluene	GW	3.00E-01	5.00E-01	6.00E-01	DUIJ81
Aniline	SW	1.20E-02	1.95E-02	6.15E-01	WEGM81
Methane, dibromochloro-	FDW	6.30E-02	8.00E-02	7.88E-01	WEST84
Benzene, ethyl-	GW	3.00E-01	3.50E-01	8.57E-01	DUIJ81
Phenol	SW	7.90E-03	8.00E-03 ^c	9.88E-01	SCHO81
Methane, dichloro-	SW	1.70E-02	1.67E-02	1.02E+00	COTR83
Methane, tribromo-	SW	1.17E-01	1.15E-01	1.02E+00	PELE81
Xylene	GW	6.00E-01	4.30E-01	1.40E+00	DUIJ81
Ethene, 1,2-dichloro-	FDW	1.20E-01	7.70E-02	1.56E+00	WEST84
Phenol, pentachloro-	SW	1.00E-02	5.00E-03	2.00E+00	WEGM79
Ethene, trichloro-	GW	1.10E+00	4.92E-01	2.24E+00	ZOET78
Methane, bromodichloro-	FDW	1.10E-01	4.50E-02	2.44E+00	WEST84

Table 2. (Continued)

Substance	Water type ^a	C _{max} (mg/L)	C _s ^b (mg/L)	Ratio C _{max} /C _s	Ref.
Carbon disulfide	SW	3.90E-03	1.40E-03	2.79E+00	KAI83
Ethane, 1,1,1-trichloro-	GW	3.10E-01	7.50E-02	4.13E+00	EPA81
Ethene, 1,1,-dichloro-	GW	9.62E-02	2.00E-02	4.81E+00	PAGE82
Methane, trichloro-	FDW	4.30E-01	8.00E-02	5.38E+00	WEST84
Trisodium nitrilotriacetate	SW	3.36E+00	6.81E-02	4.93E+01	WOOD79

^a SW = surface water, GW = ground water, FDW = finished (i.e., treated) drinking water.

^b The screening concentration is equal to the LD₅₀ multiplied by 0.0001.

^c If oral LD₅₀'s were not available, then an LD₅₀ resulting from intraperitoneal administration was used; and, if neither oral nor intraperitoneal LD₅₀'s were available, the oral LD_{Lo} was used.

concentration producing the ratio greater than 1 was obtained by sampling receiving waters below a sewage outfall. We do not believe that this substance poses a high risk for troops for the following reasons: first, the maximum concentration measured was considerably higher than the other values reported in the study (see Appendix D); second, we did not find any concentration data reported for other countries, suggesting that this material is probably not widely used; and finally, the available toxicity data suggest that it is not particularly toxic. Nixon⁷ completed a toxicity evaluation of NTA and found that a no-observed-effect level during a 90-d exposure to rats was about 200 mg/(kg·d). If we assume an animal-to-man extrapolation (safety) factor of 100 and apply Eq. 1, the equivalent drinking-water concentration representing a toxicity threshold for a 70-kg soldier consuming 15 L/d is

$$\frac{200 \text{ mg}}{\text{kg} \cdot \text{d}} \cdot \frac{70 \text{ kg}}{1} \cdot \frac{\text{d}}{15 \text{ L}} \cdot \frac{1}{100} = 9 \text{ mg/L.} \quad (3)$$

Because this value is higher than the maximum measured concentration, there is a strong possibility that even in worst-case exposure conditions, troops would not be affected.

It is also difficult to make a strong case that any of the other compounds with ratios greater than 1 pose a significant health risk to troops. For example, trichloromethane (i.e., chloroform), the compound with the second highest screening ratio, is found in many drinking waters as a product of chlorination, but it rarely reaches concentrations as high as 0.4 mg/L. Moreover, the human toxicity data indicate that dose rates of well

Table 3. Comparison of maximum concentration values in the WaterDROP data base with those used in the present study for substances with screening ratios greater than or approximately equal to unity in Table 2.

Compound	WaterDROP ^a		Our Survey		
	Water type ^b	Maximum concentration (mg/L)	Maximum concentration (mg/L)	Water type ^b	
Phenol	SW	60	>	0.006	SW
Methane, dichloro-	SW	0.03	>	0.017	SW
Phenol, pentachloro-	SW	0.4	>	0.01	SW
Xylene	SW	8.0	>	0.60	GW
Ethene, trichloro-	SW	0.1	<	1.1	GW
Ethane, 1,1,1-trichloro-	SW	0.003	<	0.3	GW
Ethene, 1,1-dichloro-	SW	0.004 ^a	<	0.096	GW
Ethene, 1,2-dichloro-	SW	0.003	<	0.12	FDW
Methane, tribromo-	SW	0.002	<	0.12	SW
Methane, bromodichloro-	FDW	0.021	<	0.11	FDW
Methane, trichloro-	FDW	0.152	<	0.43	FDW

^a WaterDROP does not list concentration data for carbon disulfide and trisodium nitrilotriacetate, nor does WaterDROP contain concentration data for Ethene, 1,1-dichloro- specifically (i.e., reported concentration is for unspecified species of dichloroethylene).

^b FDW = finished drinking water, OW = ocean water, SW = surface water, GW = ground water.

over 1 mg/(kg·d) do not produce debilitating effects.⁸ The equivalent drinking-water concentration for toxicity for the reference exposure case (i.e., a 70-kg person consuming 15 L/d) is about 5 mg/L, well above the maximum concentration of 0.4 mg/L, and therefore it is unlikely that this substance presents an unacceptable human-health risk.

As a way of checking our screening concentrations for the chlorinated methanes, ethanes, and ethenes, we compared them with toxic concentrations for water calculated from air-concentration threshold limit values (TLV's) for each of these chemicals. A TLV is an air concentration standard that is set to protect worker health for 8-h exposures to toxic substances during a 5-d work week. We converted the TLV's to an equivalent water concentration by adjusting for continuous exposures (i.e., a 7-d, 24-h exposure instead of a 5-d, 8-h exposure) and by using an inhalation volume of 10 m³ for a 70-kg man working 8 h. We also assumed that the substances were completely absorbed after inhalation

and ingestion. As an example, the TLV of chloroform is 10 parts per million by volume (ppmv or $10 \text{ m}^3/10^6 \text{ m}^3$), and it is equivalent to a concentration of 25.8 mg/L in water for our reference exposure case.

$$\text{Conc} = \frac{10 \text{ m}^3}{10^6 \text{ m}^3} \cdot \frac{10 \text{ m}^3}{\text{d}} \cdot \frac{\text{mole}}{0.022 \text{ m}^3} \cdot \frac{119.4 \text{ g}}{\text{mole}} \cdot \frac{1000 \text{ mg}}{\text{g}} \cdot \frac{5 \text{ d}}{\text{wk}} \cdot \frac{\text{wk}}{7 \text{ d}} \cdot \frac{\text{d}}{15 \text{ L}} = 25.8 \frac{\text{mg}}{\text{L}}$$

This value is more than a factor of five higher than the concentration we derived from oral exposures (i.e., 5 mg/L). The TLV and equivalent concentration in water for 1,1-dichloroethene are 5 ppmv and 10.5 mg/L, respectively. By comparison, the screening concentration calculated from LD50 data is 0.02 mg/L (see Table 2). In a similar fashion, the TLV and equivalent concentration in water for 1,1,1-trichloroethane, trichloroethene, 1,2-dichloroethene, and dichloromethane, are 350 ppmv and 1008 mg/L, 50 ppmv and 142 mg/L, 200 ppmv and 419 mg/L, and 100 ppmv and 184 mg/L, respectively. All of these equivalent concentrations are far above the screening concentrations we used. Our evaluation of the other compounds with screening ratios greater than 1 indicates that the screening concentrations are reasonable for those compounds as well.

We also used acceptable daily intake (ADI) values to check our screening concentrations. The ADI for pentachlorophenol, for example, was estimated in an EPA document⁹ to be approximately 2 mg, which translates to a drinking-water concentration of 0.1 mg/L--a factor of 20 higher than the value we used (see Table 2). The ADIs for toluene and phenol (assuming a 70-kg man) have been estimated to be 29.5 and 7 mg, respectively.^{10,11} The equivalent drinking-water concentrations are 2 and 0.5 mg/L. The value for toluene is only a factor of 4 greater than the estimated screening concentration we used; however, the maximum concentration was only 0.3 mg/L.

Data on the toxicities of the bromomethanes (i.e., dibromochloromethane, tribromomethane, and bromodichloromethane) are meager, and it is not possible to derive equivalent concentrations in water for the purpose of verifying our screening concentrations. (See the National Research Council report¹² for brief toxicity reviews of these substances.) However, we note that the bromomethanes have low water solubilities, and therefore it is conceivable that they will not reach concentrations that would be harmful.

The remaining substances with screening ratios greater than 1 (i.e., aniline, ethylbenzene, xylene, and carbon disulfide) have screening concentrations that are below concentrations calculated from the TLV's of those substances. Moreover, the screening concentrations in Table 2 for aniline (0.02 mg/L), ethylbenzene (0.35 mg/L), and xylene (0.43 mg/L) are close to the standards appearing in Table A-1 of Appendix A, that is, 0.1, 1.4, and 2 mg/L, respectively.

Screening for Organoleptic Effects

Organic compounds that impart tastes and odors to field drinking-water supplies are of concern for two basic reasons: troops are apt to become dehydrated as they reduce consumption of the aesthetically poor water, or they may seek out and consume unauthorized water supplies that are more potable, but contain toxic substances or disease-causing organisms. The process of identifying compounds that could induce these types of behavior is difficult because most of the data on odor and/or taste thresholds are based on detection thresholds rather than behavioral responses like "I could not drink this water" (see Fig. 2, Columns D and E). For screening purposes, we assume that the taste/odor thresholds are indicative of a potentially negative response. In addition, we used the minimum threshold concentration measured in water for comparisons (threshold values calculated from air data were used when threshold concentrations in water were unavailable). In Table 4 we present the screening ratios of the maximum concentrations in water (from Appendix D) to taste or odor thresholds in water (from Appendix C). Eighteen compounds had ratios greater than 1, and in Table 5 we list all of the concentration data for those compounds, arranged in alphabetical order.

From these two tables the following information about the observed concentrations can be drawn:

Benzene, 1,4-dichloro-	Only two studies reported concentrations above or equal to the organoleptic limit. The highest concentration was from a survey of New Jersey wells.
Benzene, ethyl-	Occurrence is worldwide, but the only concentration above the taste/odor threshold in Table 5 was for a landfill leachate in the Netherlands.
Biphenyl	The only concentration above the organoleptic threshold was associated with an industrial-sewage outfall into a Norwegian river. The reported concentration near this outfall was two orders of magnitude higher than the next highest reported value (see Table 5).
Carbon disulfide	Of the two concentrations in the data base, only one was above the screening concentration.

Table 4. Comparison between maximum concentrations and the minimum concentrations for taste- or odor-detection thresholds.

CASID	SUBSTANCE	MAXIMUM CONCENTRATION	TASTE/ODOR THRESHOLD	TYPE	RATIO MAXCONC/TASTEOODOR
110827	CYCLOHEXANE	2.00E-05	2.00E+02	OMH	1.00E-07
655018	PHENANTHRENE	6.40E-05	1.00E+00	OMH	6.40E-05
911212020	ANILINE	1.00E-04	1.00E+00	OMH	1.00E-04
911212020	NAPHTHALENE	1.00E-04	1.00E+00	OMH	1.00E-04
10706622	ETHANE, 1,2-DICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
933372927	PHENOL, 2,3,6-TRICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
110552227	BENZALDEHYDE	1.00E-04	1.00E+00	OMH	1.00E-04
1108741	BENZENE, HEXACHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
75014	ETHENE, CHLORO-(VINYLCHLORIDE	1.00E-04	1.00E+00	OMH	1.00E-04
5499990	ETHENE, 1,2-DICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
87683	BUTADIENE, HEXACHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
108601	ETHER, BIS(2-CHLOROISOPROPYL)-	1.00E-04	1.00E+00	OMH	1.00E-04
108907	BENZENE, CHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
98953	BENZENE, NITRO-	1.00E-04	1.00E+00	OMH	1.00E-04
5412334	METHANE, TETRACHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
753316	BENZENE, 1,1-DICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
750092	ETHENE, TRICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
8076646	METHANE, DICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
7533924	PHENOL, PENTACHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
7509024	METHANE, TRIBROMO-	1.00E-04	1.00E+00	OMH	1.00E-04
5589024	PHENOL, 2,2,3-TETRACHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
996994	PHENOL, 2,4,5-TRICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
9966501	BENZENE, 1,2-DICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
9257722	PHENOL, 3,4-DICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
1221844	BIPHENYL	1.00E-04	1.00E+00	OMH	1.00E-04
1271844	ETHENE, TETRACHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
8880622	PHENOL, 2,4,6-TRICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
5837888	PHENOL, 2,5-DICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
751500	CARBON DISULFIDE	1.00E-04	1.00E+00	OMH	1.00E-04
120832	PHENOL, 2,4-DICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
8876400	PHENOL, 2,6-DICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
1088883	TOLUENE	1.00E-04	1.00E+00	OMH	1.00E-04
777474	CYCLOPENTADIENE, HEXACHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
108414	PHENOL	1.00E-04	1.00E+00	OMH	1.00E-04
676633	BENZENE, ETHYL-	1.00E-04	1.00E+00	OMH	1.00E-04
955578	METHANE, TRICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
788678	PHENOL, 2-CHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
1064482	PROPANE, 1,2-DICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
1064482	PHENOL, 4-CHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
108430	BENZENE, 1,4-DICHLORO-	1.00E-04	1.00E+00	OMH	1.00E-04
	PHENOL, M-CHLORO-	6.00E-03	1.00E+00	OMH	6.00E-03

* O = ODOR
 T = TASTE
 M = MINIMUM
 A = AVERAGE
 W = WATER
 C = CALCULATED.

Table 5. Comparison between screening concentrations based on LD₅₀ values and all concentration data reported for those organic chemicals that appear in Table 4 and have a maximum concentration to taste- or odor-detection threshold ratio greater than unity.

Table 5. (Continued)

CASID	SUBSTANCE	TYPE*	REPORTED CONCENTRATIONS MG/L	SCREENING	# SAMP	REFERENCE	PLACE
75150	CARBON DISULFIDE	FDW	4.80E-06	1.40E-02	1	KYES82	FINLAND
77474	CYCLOPENTADIENE, HEXACHLORO-			1.13E-01	17	KAIS83	NORT-HY
127184	ETHENE, TETRACHLORO-			8.10E+00	98	COTR83	NEW YORK
					2	SCHH79	CANADA, ONTARIO
					3	SCHH79	UNITED STATES
					4	SCHH79	SWITZERLAND
					5	SCHH79	SWITZERLAND
					6	SCHH79	GULF OF MEXICO
					7	SCHH79	SWITZERLAND
					8	SCHH79	SWITZERLAND
					9	SCHH79	AUSTRALIA
					10	SCHH79	NEW YORK
					11	SCHH79	NETHERLANDS
					12	SCHH79	CHINA
					13	SCHH79	EGYPT
					14	SCHH79	SOUTH AFRICA
					15	SCHH79	NETHERLANDS
					16	SCHH79	SOUTH AFRICA
					17	SCHH79	SOUTH AFRICA
					18	SCHH79	SOUTH AFRICA
					19	SCHH79	SOUTH AFRICA
					20	SCHH79	SOUTH AFRICA
					21	SCHH79	SOUTH AFRICA
					22	SCHH79	SOUTH AFRICA
					23	SCHH79	SOUTH AFRICA
					24	SCHH79	SOUTH AFRICA
					25	SCHH79	SOUTH AFRICA
					26	SCHH79	SOUTH AFRICA
					27	SCHH79	SOUTH AFRICA
					28	SCHH79	SOUTH AFRICA
					29	SCHH79	SOUTH AFRICA
					30	SCHH79	SOUTH AFRICA
					31	SCHH79	SOUTH AFRICA
					32	SCHH79	SOUTH AFRICA
					33	SCHH79	SOUTH AFRICA
					34	SCHH79	SOUTH AFRICA
					35	SCHH79	SOUTH AFRICA
					36	SCHH79	SOUTH AFRICA
					37	SCHH79	SOUTH AFRICA
					38	SCHH79	SOUTH AFRICA
					39	SCHH79	SOUTH AFRICA
					40	SCHH79	SOUTH AFRICA
					41	SCHH79	SOUTH AFRICA
					42	SCHH79	SOUTH AFRICA
					43	SCHH79	SOUTH AFRICA
					44	SCHH79	SOUTH AFRICA
					45	SCHH79	SOUTH AFRICA
					46	SCHH79	SOUTH AFRICA
					47	SCHH79	SOUTH AFRICA
					48	SCHH79	SOUTH AFRICA
					49	SCHH79	SOUTH AFRICA
					50	SCHH79	SOUTH AFRICA
					51	SCHH79	SOUTH AFRICA
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					69	SCHH79	SOUTH AFRICA
					70	SCHH79	SOUTH AFRICA
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					72	SCHH79	SOUTH AFRICA
					73	SCHH79	SOUTH AFRICA
					74	SCHH79	SOUTH AFRICA
					75	SCHH79	SOUTH AFRICA
					76	SCHH79	SOUTH AFRICA
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Table 5. (Continued)

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Table 5. (Continued)

CASID	SUBSTANCE	TYPE*	REPORTED CONCENTRATIONS MG/L	SCREENING SAMPLE	# REFERENCE	PLACE
SH	SH	FDW	7.00E+04	1 TRUS80	PERU	
SH	SH	FDW	7.00E+04	1 HEST84	CHINA	
SH	SH	FDW	7.50E+04	321 HEST84	UNITED STATES	
SH	SH	FDW	8.00E+04	280 HEST84	UNITED STATES	
SH	SH	FDW	9.00E+04	1 TRUS80	VENEZUELA	
SH	SH	FDW	1.00E+05	1 VAND81	NETHERLANDS	
SH	SH	FDW	1.20E+05	1 TRUS80	EGYPT	
SH	SH	FDW	1.29E+05	1 TRUS80	BRAZIL	
SH	SH	FDW	1.49E+05	1 TRUS80	THAILAND	
SH	SH	FDW	1.50E+05	1 TRUS80	PHILIPPINES	
SH	SH	FDW	1.55E+05	1 TRUS80	UNITED STATES	
SH	SH	FDW	2.30E+05	158 HEST84	HICAPAGUA	
SH	SH	FDW	2.90E+05	1 HEST84	UNITED STATES	
SH	SH	FDW	3.00E+05	184 HEST84	NETHERLANDS	
SH	SH	FDW	3.00E+05	1 VAND81	NEW YORK	
SH	SH	FDW	3.00E+05	1 COTR83	UNITED STATES	
SH	SH	FDW	3.00E+05	1 VAND81	NETHERLANDS	
GW	GW	GW	3.00E+05	1 VAND81	NETHERLANDS	

Note: Screening concentration is based on LD50 data.

* FDW = finished drinking water.

GW = ground water.

SW = surface water.

OW = ocean water.

Cyclopentadiene, hexachloro-	The only concentration value we were able to obtain was above the organoleptic threshold.
Ethene, tetrachloro-	Its occurrence is worldwide. The highest concentration was for a U.S. surface water. The other values were below the screening concentration.
Methane, trichloro-	The highest concentration values are from the U.S., but worldwide values are not significantly lower.
Phenol	All but one of the values listed in our basic source data, Table D-1, Appendix D, are from Norway. Organoleptic response would be zero at these concentrations; however, we did find higher values in the WaterDROP data base for waters in the U.S. The highest was 60 mg/L at the outlet of an industrial discharge. This value would definitely be above the taste/odor threshold. (WaterDROP data, as explained previously, were used for comparison.)
Phenols, chloro- (mono-, di-, trichloro-)	Most of the values were from a study of the Rhine River in the Netherlands.
Phenol, pentachloro-	All surface-water monitoring data we surveyed were from the Netherlands or Japan. The largest concentration in WaterDROP is an order of magnitude higher than our survey data.
Propane, 1,2-dichloro-	All values are for tap waters in North America.
Toluene	It is found worldwide, but the problem concentration was for a landfill leachate in the Netherlands.

We can place most of the compounds with ratios less than 0.1 in Table 4 into two classes: phenols and their chlorinated homologs and chlorinated hydrocarbons. The compounds with ratios of 0.1 to 1.0 are also primarily chlorinated hydrocarbons and phenols. Tetrachloroethene, 1,2-dichloropropane, trichloroethene, dichloromethane, and dibromomethane are found in many of the same studies. Toluene (i.e., methylbenzene) and

ethylbenzene are found in the same studies. Likewise, all chlorinated phenols are found together. We would expect the total olfactory contributions of these combinations to be greater than the single contributions.

The compounds with the greatest worldwide distributions (see Table 5) are ethylbenzene, tetrachloroethene, trichloromethane, and toluene. Of these four substances, the one with the highest screening ratio was trichloromethane, with a ratio of 4.3. It was followed by ethylbenzene (3.0), toluene (2.5), and tetrachloroethene (1.25). None of the measured concentrations is greatly above the detection thresholds, and therefore these substances may not actually cause adverse organoleptic responses. Our data on the chlorinated phenols were derived from a single study of the Rhine River; however, phenolic compounds can be expected in other similar rivers receiving industrial discharges (we will discuss the phenolic compounds again in a later section).

An important source of uncertainty in the screening for potential organoleptic effects has been the lack of adequate psychometric data on the kinds of responses expected at the contaminant concentrations presented. If the threshold concentrations we have used for screening are far below levels that would actually cause a soldier to refuse water, then none of these substances truly represents a problem. To rectify this situation, we recommend that taste panels comprised of soldiers be used to quantify the behavioral responses to varying concentrations of the organic solutes noted above.

PREDICTED ORGANIC-SOLUTE CONCENTRATION MAXIMA IN THE SURFACE WATERS OF REPRESENTATIVE FOREIGN COUNTRIES

We recognize the fact that measurement bias may play a role in the screening comparisons we performed using observed-maximum concentrations. Therefore, to compensate for such possible bias, we augmented our initial screening process with one that uses predicted concentrations of the following organic substances:

- Acenaphthene,
- Acrolein,
- Acrylonitrile,
- Chloromethane,
- Cyanide,

- 2,4-Dinitrophenol,
- Oil and grease,
- Pentachlorophenol,
- Phenol, and
- Phenol (4AAP)^a.

These are major contaminants that are likely to be present in the waste waters from 13 major industrial sources in foreign countries. The industrial sources include: (1) aluminum forming, (2) coal mining, (3) copper forming, (4) foundries, (5) iron and steel mills, (6) leather tanning, (7) metal finishing, (8) nonferrous metal production, (9) ore mining, (10) organic chemical/plastic production, (11) petroleum refining, (12) pulp and paper production, and (13) textile manufacturing.

To predict the maximum concentrations in surface water of the organic substances listed above, we used a model that combines data for (1) the annual release of each of the organic chemicals into wastestreams by the U.S. industries that are in the previously mentioned 13 industrial categories, with data for (2) the annual production of the manufactured/mined material from each of the 13 industrial categories in five representative foreign countries and in the U.S., and (3) country-specific hydrologic data. Comparison between these predicted maximum concentrations in surface water and the corresponding estimates of threshold concentrations for toxic effects (based on 70-kg military personnel consuming water at a rate up to 15 L/d) or organoleptic responses will augment the screening for the set of organic compounds that could pose a human health risk to military personnel consuming field water in foreign countries.

Our approach for estimating the concentration of an arbitrary chemical in the surface water of a given country is based on the influence diagram shown in Fig. 4. This figure is based in part on the concepts described by Mackay.¹³ For our purposes, for example, the concentration of an organic compound in a river, lake, or estuary is related to (1) the amount of the compound in industrial effluents (both direct and indirect), (2) the advection (e.g., horizontal transport) properties for receiving waters, and (3) the attenuation of the organic compound's concentration in water by means of biogeochemical processes. The contribution of industrial effluents to organic-chemical pollution of surface waters is estimated by considering (1) the types of industries that release the compound into wastestreams, (2) the most prominent organic chemicals released into the wastestreams (per unit of production) by each industry, and (3) the level of output of

^aThe designation 4AAP refers to the method of detection, which involves the reaction of phenolic compounds with 4-aminoantipyrine (i.e., 4AAP).

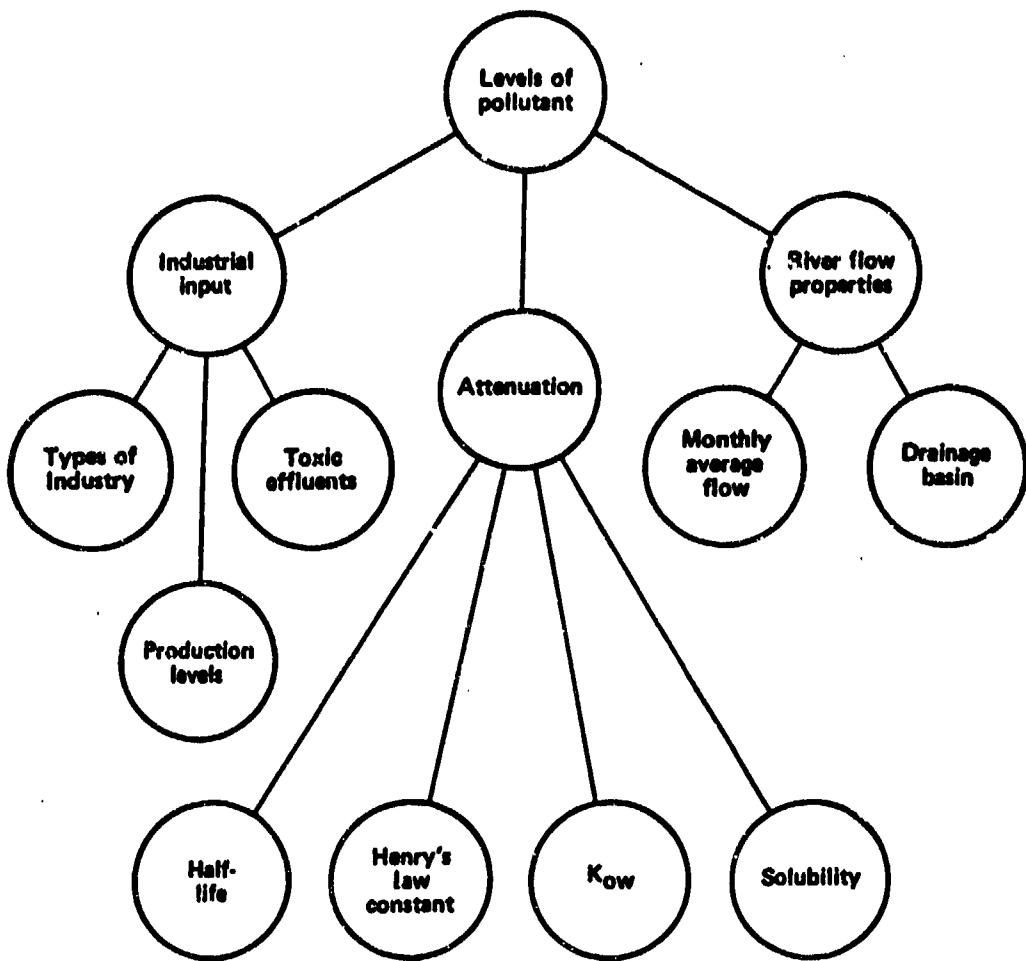


Figure 4. Influence diagram for processes that affect the concentration of organic solutes in surface waters.

manufactured/mined material each industry produces. The volume of surface water available for diluting the released organic chemicals is determined using river-flow properties (e.g., average-flow volume monthly). The physicochemical properties of the organic compounds released provide information on the potential attenuation of concentration by chemical decay (biodegradation, photolysis, hydrolysis, oxidation, and volatilization), sorption by sediments, and uptake by biomass. However, in order to simplify our calculation and provide a conservative upper bound for our concentration estimate, attenuation as a result of these chemical processes was excluded from our model. Dilution by advection within the water system, however, was included in the model. Figure 5 provides an illustration of a national water system as it is viewed for the purposes of this model.

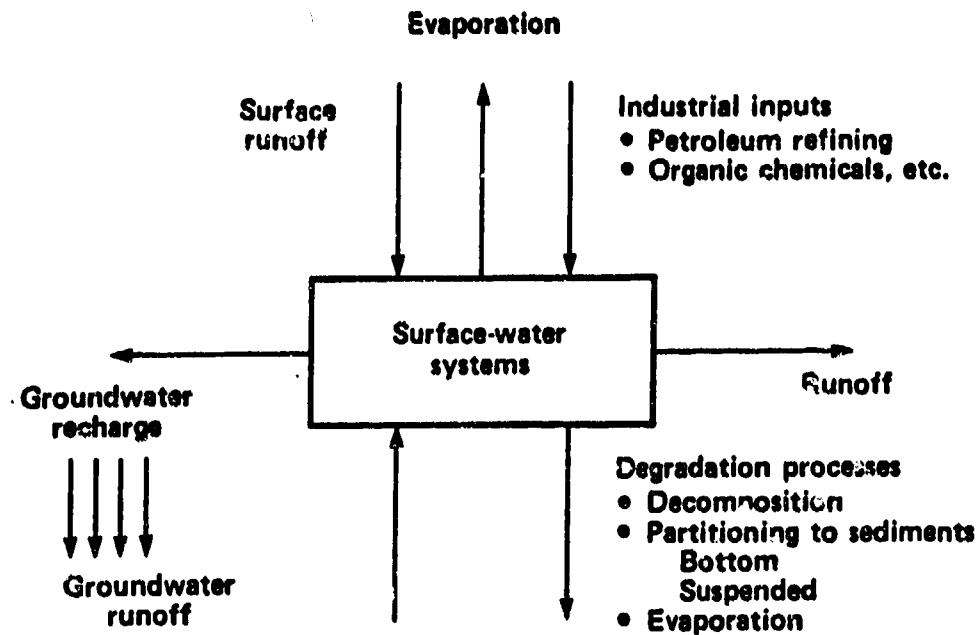


Figure 5. A schematic view of a national water system for use in screening organic solutes likely to be at potentially toxic levels.

The screening methodology was applied to each of the five representative countries according to the following mathematical expression:

$$C_{i,m} = \frac{1}{R_m} \sum_{j=1}^n F_{i,j} \cdot P_{j,m},$$

where

- $C_{i,m}$ - the concentration of chemical compound, i (g/L), in the surface waters of country, m ;
- R_m - the discharge of the major rivers (L/y) in country, m , that are likely to be receiving industrial wastestreams;
- $F_{i,j}$ - the amount of chemical, i (g/y), contained in the raw-effluent wastestream generated annually by industry, j , in the U.S. (The choice of raw-effluent wastestream instead of treated-effluent wastestream tends to provide added conservatism to this figure; this assumption also is realistic for most developing countries); and

$P_{j,m}$ - the ratio between the annual manufacturing output produced nationally for industry, j , in country, m , and the same production-output value for industry, j , in the U.S. We define this ratio as the production-output factor (dimensionless) for industry, j , in country, m .

Statistics compiled by the United Nations¹⁴ concerning the annual manufacturing output produced nationally in a particular country by a specific industrial category were used to derive the production-output factor ($P_{j,m}$). Data on the amounts of the organic chemicals of interest contained in the raw-effluent wastestreams generated annually by an industry category in the U.S. (i.e., $F_{i,j}$) were obtained from a U.S. EPA-sponsored study concerning the discharges of 86 organic contaminants released from 24 industries in the U.S.¹⁵ The surface-water volume available in each country (R_m) for dilution of the organic chemicals contained in the raw-effluent wastestreams generated annually by the combination of all 13 industrial categories was obtained from a reference work edited by van der Leeden¹⁶; these figures correspond to the volumes of major surface-water systems in each country that are likely to receive industrial wastestreams, and therefore they are not necessarily equal to the total surface runoff in each country.

Once the estimated concentration of a specific organic chemical is calculated for a particular representative country ($C_{i,m}$), based on the industrial mix and the receiving-water flow, the chemicals are ranked for each country, using the screening-criteria formula:

$$S_{i,m} = \frac{C_{i,m}}{T_i} ,$$

where

- $S_{i,m}$ - screening-criteria ratio (dimensionless) for chemical, i , in country, m ,
- $C_{i,m}$ - concentration of chemical compound, i (mg/L), in the surface waters of country, m , and
- T_i - an estimate of the threshold concentration (mg/L) in water of chemical, i , for toxicity or organoleptic effects, based on 70-kg military personnel consuming water at a consumption rate of up to 15 L/d.

Table 6. Production-output factors^a for estimating source terms from the 13 industrial/mining categories that we consider to be major sources of organic-chemical pollution in foreign countries.

Industry	Country				
	Egypt	Iran	Israel	Thailand	Turkey
Production factors					
Aluminum forming	2.00E-03	1.60E-03	0	0	8.30E-03
Coal mining	0	1.60E-03	0	9.80E-04	7.50E-03
Copper forming	0	0	0	0	1.10E-02
Foundries	7.20E-03	8.13E-05	8.10E-04	2.60E-03	1.50E-02
Iron and steel	7.50E-03	0	9.90E-04	3.20E-03	1.70E-02
Leather tanning	0	4.50E-02	0	0	1.10E-01
Metal finishing	1.80E-02	3.80E-02	3.90E-03	2.80E-03	2.60E-02
Nonferrous metals	0	0	0	0	4.30E-03
Ore mining	1.40E-02	7.20E-03	1.60E-05	1.30E-03	4.50E-02
Organics/plastics	4.90E-04	4.70E-05	1.30E-03	3.90E-06	5.80E-03
Petroleum refining	1.80E-02	3.40E-02	1.40E-02	1.10E-02	2.00E-02
Pulp and paper	1.20E-03	7.80E-04	1.10E-03	4.60E-03	6.80E-03
Textiles	0	2.60E-02	0	1.50E-01	4.00E-02

^a Production-output factors are calculated by dividing the annual manufacturing or mining output from an industrial/mining category for a foreign country by the same value for the equivalent industrial/mining category in the U.S. The amount of organic-chemical pollutant contained in the raw-effluent wastestreams for all 13 industrial/mining categories in a foreign country is then the sum of the product of the production-output factor and the amount of organic-chemical pollutant in the raw-effluent wastestreams generated by each industrial/mining category in the U.S.

Application of the Model to Five Representative Countries

The model described above was applied to the following countries: Egypt, Iran, Israel, Thailand, and Turkey. These countries were selected because they possess the wide range of industrial and climatic conditions that are most likely to be encountered in foreign countries. Table 6 lists the production-output factors for the thirteen industrial categories that we used to scale the level of organic-chemical pollutant contained in the raw-effluent wastestreams generated by these industries in the five foreign countries just mentioned. Table 7 lists the amounts of the pollutants contained in the raw-effluent wastestreams generated annually in the U.S. by each of the 13 industrial categories. Table 8 presents the average and low-dilution volumes provided annually by major rivers

Table 7. U.S. production of organic by-products in g/y for each industrial category.

Industry	Organic Substances							
	Acenaph-thene	Acrolein	Acrylo-nitrile	Chloro-methane	Cyanide	2,4-Dinitro-phenol	Penta-chloro-phenol	Phenol (4AAP) ^a
Aluminum forming						1.16E+06	8.58E+08	8.65E+05
Coal mining						2.66E+06		8.87E+07
Copper forming						2.80E+06	4.59E+11	2.13E+08
Foundries	1.43E+07					1.10E+06	3.13E+10	1.14E+07
Iron and steel		5.46E+07					2.93E+11	2.55E+09
Leather tanning	7.43E+05					2.39E+06	6.00E+06	1.80E+10
Metal finishing						1.43E+10	1.98E+10	1.39E+10
Nonsferrous metals	2.25E+07					1.21E+08	6.01E+06	1.60E+08
Ore mining						1.17E+09		2.51E+08
Organics/plastics	5.24E+09	1.04E+10	6.89E+09	1.87E+08	1.79E+09	6.67E+07		2.52E+08
Petroleum refining	8.14E+07	3.02E+05				5.45E+07		5.66E+06
Pulp and paper						8.41E+07	4.60E+08	1.77E+10
Textiles		1.85E+07				1.37E+07		7.85E+06
							6.49E+10	9.48E+05
							3.73E+10	5.90E+08
							4.87E+07	9.70E+09
								2.12E+08
								2.01E+07

^aThe designation 4AAP refers to the method of detection, which involves the reaction of phenolic compounds with 4-aminoantipyrine (i.e., 4AAP).

Table 8. Annual average and low dilution volumes provided by major rivers in each of the candidate countries.

Country	Dilution volume ^a (L/y)	
	Low	Average
Egypt	2.21E+13	8.20E+13
Iran	3.15E+11	9.46E+12
Israel	9.10E+10	1.96E+12
Thailand	5.20E+13	2.90E+14
Turkey	1.40E+13	4.00E+13

^a The low dilution volume was calculated by multiplying the lowest monthly flow by 12.

Table 9. Annual mass discharges of the major organic contaminants released into the raw-effluent wastestreams of all 13 industrial/mining categories in each of five representative countries.

Contaminant	Country				
	Egypt	Iran	Israel	Thailand	Turkey
Mass discharged, kg/y					
Acenaphthene	4.13E+06	3.05E+06	7.96E+06	9.53E+05	3.24E+07
Acrolein	5.08E+06	4.97E+05	1.35E+07	4.37E+04	6.01E+07
Acrylonitrile	3.79E+06	8.06E+05	9.02E+06	2.98E+06	4.16E+07
Chloromethane	9.14E+04	8.77E+03	2.43E+05	7.28E+02	1.08E+06
Cyanide	2.61E+08	5.47E+08	5.92E+07	4.31E+07	3.88E+08
2,4-Dinitrophenol	8.32E+06	1.57E+07	6.52E+06	5.07E+06	9.54E+06
Oil and grease	6.15E+09	9.48E+09	1.78E+09	7.73E+09	1.92E+10
Pentachlorophenol	2.07E+05	6.68E+05	9.22E+04	2.17E+06	1.83E+06
Phenol	1.72E+08	2.90E+07	5.13E+07	7.46E+07	4.79E+08
Phenol (4AAP) ^a	3.04E+08	3.30E+08	1.52E+08	1.60E+08	4.86E+08

^a Phenol (4AAP) includes soluble phenolic compounds.

in each of the five representative countries. Table 9 contains the estimated total amount of each of the organic-chemical pollutants generated in each country from the combination of all 13 industrial categories. An estimate of the maximum and mean concentrations for each of the pollutants of interest in the surface waters of each of the five representative countries are presented in Table 10. Finally, Table 11 contains the values representing toxicity or organoleptic threshold concentrations (T_i) and screening-criteria ratios ($S_{i,m}$) for each of the organic chemicals of interest.

According to the screening-criteria ratios presented in Table 11, dissolved oil and grease is of potential concern in virtually all foreign countries. The screening-criteria value for oil and grease was computed using the Soviet taste/odor standard of 0.1 mg/L for crude oil (high sulfur) and kerosene reported by Bedding *et al.*¹⁸ The importance of oil and grease is not surprising because oil and grease are major components of many industrial effluents prior to wastewater treatment. We were able to obtain some water-quality data that corroborate this prediction from our screening. For example, Moursy¹⁹ measured concentrations of oil and grease in the Nile River that were typically between 1 and 30 mg/L. The highest of these concentrations were recorded near the major industrialized areas along the river. In another study Cordero *et al.*²⁰ sampled water from the Bermudez River in Costa Rica at three separate locations and measured oil and grease levels ranging from approximately 30 to 50 mg/L. This river also received effluents from various industrial sources.

In addition to oil and grease posing potential problems for military personnel from an organoleptic standpoint, these hydrocarbons can interfere with the operation of the Reverse Osmosis Water Purification Unit (ROWPU). Specifically, oil and grease can create a film on the reverse osmosis membrane and thus decrease its ability to desalinate water.

The other organic chemicals of potentially greatest concern to U.S. military personnel in foreign countries are the phenolic compounds detected by their reaction with 4-aminoantipyrine (i.e., 4AAP). The screening-criteria values are all greater than one for this class of organic compounds for each of the five representative countries. These phenolic compounds are not a problem in drinking water from a toxicological standpoint because the WHO limit for 2,4,6-trichlorophenol is an organoleptic limit.

Generally, Israel is the country predicted to have the highest concentrations in their surface waters (see Table 10) of the organic chemicals of interest. However, the predicted concentrations that appear in Table 10 are very conservative because we have assumed that there is no pretreatment (e.g., chlorination) of raw-effluent wastestreams, and we have used the low-dilution volumes for receiving waters.

Table 10. The estimated maximum^a and mean concentrations of each of the major organic chemicals in the surface waters of each of five representative countries.

Contaminant	Country						Concentration (mg/L)	
	Egypt		Iran		Israel			
	Max.	Mean	Max.	Mean	Max.	Mean		
Acenaphthene	1.87E-04	5.04E-05	9.67E-03	3.22E-04	8.76E-02	4.06E-03	1.83E-05	
Acrolein	2.30E-04	6.19E-05	1.58E-03	5.25E-05	1.48E-01	6.87E-03	8.40E-07	
Acrylonitrile	1.71E-04	4.62E-05	2.55E-03	8.52E-05	9.93E-02	4.60E-03	5.73E-05	
Chloromethane	4.14E-06	1.11E-06	2.78E-05	9.27E-07	2.67E-03	1.24E-04	1.40E-08	
Cyanide	1.18E-02	3.18E-03	1.73E+00	5.78E-02	6.52E-01	3.02E-02	8.29E-04	
2,4-Dinitrophenol	3.77E-04	1.01E-04	4.96E-02	1.66E-03	7.18E-02	3.33E-03	9.75E-05	
Oil and grease	2.78E-01	7.50E-02	3.00E+01	1.00E+00	1.96E+01	9.07E-01	1.49E-04	
Pentachlorophenol	9.35E-06	2.52E-06	2.12E-03	7.06E-05	1.02E-03	4.71E-05	4.17E-06	
Phenol	7.81E-03	2.10E-03	9.18E-02	3.06E-03	5.65E-01	2.62E-02	1.43E-03	
Phenol (4AAP) ^b	1.37E-02	3.70E-03	1.05E+00	3.49E-02	1.68E+00	7.77E-02	3.08E-03	

^a The maximum concentration is calculated from a dilution volume by multiplying the lowest monthly flow volume by 12. The mean is calculated from annual average flows.

^b Phenol (4AAP) includes soluble phenolic compounds.

Table 11. Toxicity- or organoleptic-threshold concentrations in water (T_i , based on 70-kg military personnel consuming up to 15 L/d of drinking water) and screening-criteria ratios ($S_{i,m}$, calculated by dividing the estimated maximum concentration in the water of a particular country, $C_{i,m}$, by T_i) for each of the major organic chemicals (i) in each of five representative countries (m).

Contaminant	Screening concentration (mg/L)	Country Israel Thailand Turkey Concentration ratios				
		Egypt	Iran			
Acenaphthene	2.00E-02 ^a	9.35E-03	4.83E-01	4.38E+00	9.17E-04	1.16E-01
Acrolein	3.20E-01 ^a	7.18E-04	4.92E-03	4.63E-01	2.63E-06	1.34E-02
Acrylonitrile	2.00E+00 ^a	8.57E-05	1.28E-03	4.96E-02	2.87E-05	1.49E-03
Chloromethane	2.00E-03 ^a	2.07E-03	1.39E-02	1.34E+00	7.00E-06	3.86E-02
Cyanide	2.00E+00 ^b	5.90E-03	8.65E-01	3.26E-01	4.14E-04	1.38E-02
2,4-Dinitrophenol	3.00E-02 ^a	1.26E-02	1.65E+00	2.39E+00	3.25E-03	2.27E-02
Oil and grease	1.00E-01 ^c	2.78E+00	3.00E+02	1.96E+02	1.49E+00	1.37E+01
Pentachlorophenol	5.00E-03 ^d	1.87E-03	4.24E-01	2.04E-01	8.34E-03	2.62E-02
Phenol	3.50E+00 ^a	2.23E-03	3.62E-02	1.61E-01	4.10E-04	9.77E-03
Phenol (4AAP) ^e	1.00E-04 ^f	1.38E+02	1.04E+04	1.68E+04	3.08E+01	3.47E+02

^a Lowest health standard or guideline (see Appendix A).

^b Interim value recommended by Scofield *et al.* for field-water supplies.¹⁷

^c Taste/odor standards of USSR for oil and kerosene.¹⁸

^d Value calculated from oral LD50 (see Table 2).

^e Phenol (4AAP) includes soluble phenolic compounds.

^f WHO limit for 2,4,6-trichlorophenol (see Appendix A).

BIOCHEMICAL COMPOUNDS RELEASED BY ALGAE AND ASSOCIATED MICROORGANISMS

The ubiquitous aquatic microorganisms, cyanobacteria (blue-green algae) and actinomycetes (Gram-positive filamentous bacteria that grow in close association with cyanobacteria), have been identified as the source of taste- and odor-producing biochemical compounds in surface waters, particularly drinking-water reservoirs (Krasner *et al.*, 1981).²¹ Furthermore, there is even circumstantial evidence suggesting that a causal relationship exists between otherwise unexplainable outbreaks of adverse health effects in human populations and the presence of toxic biochemicals released by

cyanobacteria into public drinking-water supplies.²²⁻²⁷ Therefore, in addition to the organic chemicals previously discussed, we also assessed the significance of these natural organic compounds from the perspective of military field-water quality.

Our assessment revealed that there are two taste- and odor-causing metabolites of cyanobacteria and actinomycetes--geosmin and 2-methylisoborneol (MIB)--that can be of military concern in field water, especially when algal blooms are present. There are two reasons that justify this conclusion. First, these metabolites can occur in field water at concentrations above organoleptic thresholds. For example, according to a survey cited by Zoeteman (1981)²⁸ comparing the maximum concentration measured in drinking water of taste-impairing substances with their odor-threshold concentration (defined as the concentration at which 50% of the subjects can detect the odor of the substance), the ratios of maximum concentration to odor-threshold concentration were among the greatest for geosmin and MIB (i.e., 1.5 - 0.03 µg/L of water/0.02 µg/L of water). Second, these biologically released substances resist oxidation and therefore are difficult to remove by standard water-treatment processes such as chlorination (Krasner *et al.*, 1981).²¹ Consequently, military personnel exposed to field water containing maximum concentrations of geosmin and MIB may refuse to consume such water based on objectionable organoleptic properties (i.e., taste and odor) and therefore can become susceptible to the performance-degrading health effects associated with dehydration. Moreover, chlorination, which is the water-treatment technique most commonly available in the field, normally is ineffective in destroying these compounds.

Another group of biochemicals that may be of military concern are the alkaloid, lipopolysaccharide, and polypeptide metabolites that are released by cyanobacteria. These natural organic substances have been associated with the death of animals, especially cattle, and are implicated as being toxic to man (Carmichael, 1981).²⁹ Consequently, the potential for performance-degrading effects from human exposure to these substances should be evaluated further.

SUMMARY AND RECOMMENDATIONS

Our screening effort has addressed substances that could potentially cause toxic or organoleptic effects in troops that drink field water. To minimize the omission of substances that might adversely affect troops, we made conservative assumptions for screening for those organic chemicals that could be present in field water at concentrations that could produce organoleptic effects or toxicity in military personnel forced to consume up to 15 L/d of field water. Moreover, we assumed that no treatment

would occur prior to water consumption. From our comparison between reported maximum-observed concentrations and threshold concentrations for toxicity (based on a 15-L/d consumption rate for a 70-kg individual), we conclude that there is a very low probability that organic solutes in field water will cause direct, debilitating effects in troops. However, this assumes that troops follow existing doctrine regarding the placement of water-supply points. Siting a water point directly below a sewage outfall on a stream or river, for example, greatly enhances the risk of health effects. Likewise, the use of a well that is in the immediate vicinity of actual or possible surface industrial contamination poses an increased health risk. Avoiding these obvious situations is a key precaution in the management of health risks from all contaminants of field water.

We have identified several compounds that have the potential for causing organoleptic effects (e.g., objectionable taste or odor). Among the most important compounds in this group are trichloromethane, ethylbenzene, toluene, and tetrachloroethylene because they have the greatest worldwide distribution. In addition, chlorinated phenols, as well as oil and grease, could impair the potability of field water. Our screening for organoleptic effects, however, utilized concentrations for taste- and odor-detection thresholds instead of concentrations related to a behavioral response, such as refusal to drink poor-tasting water. We therefore recommend that taste panels comprised of groups of soldiers be used to quantify the relationship between the concentrations of these substances, an organoleptic property, and various behavioral responses (see, for example, Daniels and Layton, 1988³⁰). This research could provide a data base that would support a more definitive analysis for determining the organic chemicals likely to impair the potability of field water. An important issue that has emerged is the effect that oil and grease could have on the operation of a ROWPU. Studies are needed to determine the concentrations of oil and grease that could impair the efficiency of reverse osmosis membranes.

Finally, we indicate that compounds released into water by the aquatic microorganisms, cyanobacteria and actinomycetes, can also be of particular military concern. These substances fall into two categories: (1) those that impair the taste and odor of drinking water and (2) those that could produce toxic health effects following ingestion or nonconsumptive exposure. Geosmin and MIB fall into the first category and alkaloid, lipopolysaccharide, and polypeptide toxins belong to the second one. Because of the potential for algal blooms in surface waters, we recommend that available data on the organoleptic and toxic properties of these metabolites be evaluated carefully so that consideration can be given to developing criteria and recommendations for their standards in field water.

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APPENDIX A

HEALTH STANDARDS AND GUIDELINES FOR ORGANIC WATER CONTAMINANTS

As a starting point for our screening analyses of organic contaminants that could pose health problems, we compiled relevant health standards and guidelines developed by domestic as well as foreign organizations. Table A-1 summarizes the results of our regulatory review. Included in the table are short-term (approximately 10 d or less) and long-term (chronic exposure) standards. For example, a 7-d standard is expressed as 7d, followed by a slash and the standard in mg/L (e.g., 7d/0.03). We have also listed substances that have been identified as hazardous by different organizations. For a number of substances we calculated an equivalent drinking-water concentration from Acceptable Daily Intakes (ADIs).

Table A-1. Regulatory status of organic compounds (excluding pesticides).

CAS#	Substance	Formula	EPA pp	EPA advis*	NAS snarl*	NAS 3d1	WHO std	Soviet std	WPS tox	Other
			mg/l							
83329	acetophenone	C12H10	x							0.02
203962	acetylphenylene	C12H8	x							
141786	acetic acid, ethyl ester	C4H8O2								
79209	acetic acid, methyl ester	C3H6O2								
106054	acetic acid, vinyl ester	C4H6O2								
36662	acetophenone	C9H10								
107028	acrolein	C3H4O	x							
79061	acrylamide	C3H5NO								
79107	acrylic acid	C3H4O2								
167131	acrylonitrile	C3H3N	x							
111693	adiponitrile	C6H10N2								
62533	anilin	C6H7N								
163429	anilin, 2-chloro-	C6H5Cl								
99092	anilin, 2-nitro-	C6H5NO2								
88744	anilin, 4-nitro-	C6H5NO2								
106478	anilin, p-chloro-	C6H5Cl								
100016	aniline, p-nitro-	C6H5NO2								
106663	anisole	C7H10								
71432	benzene	C6H6	x							
106997	benzene, chloro-	C6H5Cl	x							
100414	benzene, ethyl-	C6H10	x							
110741	benzene, hexachloro-	C6C16	x							
36953	benzene, nitro-	C6H5NO2	x							
577599	benzene, o-diisopropyl-	C12H10								
608935	benzene, pentachloro-	C6C15								0.074
121733	benzene, 1-chloro-3-nitro-	C6H4ClNO2								
100005	benzene, 1-chloro-4-nitro-	C6H4ClNO2								
95501	benzene, 1,2-dichloro-	C6H2Cl2	x							
95943	benzene, 1,2,4,5-tetrachloro-	C6C2Cl4	x							
541731	benzene, 1,3-dichloro-	C6H4Cl2	x							
106467	benzene, 1,4-dichloro-	C6H4Cl2	x							
92075	benzidine	C12H10	x							
91941	benzidine, 2,3'-dichloro-	C12H10Cl2	x							
56553	benzo[a]anthracene	C18H12	x							
36126	biphenyl	C22H12	x							
205992	benzo[b]fluoranthene	C20H12	x							
191242	benzo[ghi]perylene	C22H12	x							
207069	benzofuran, 2-phenyl-	C20H12	x							
92524	biphenyl	C12H10								
2304669	butachlor	C17H26ClNO2								
87683	butadiene, hexachloro-	C4C16	x							
79333	buten-2-one	C4H8O								
										15.
										car
										car
										haz

Table A-i. (Continued).

cas#	Substance	formula	EPA pp	EPA adv/s*	MS smr1*	MS adv	MS std	MS var	MS var	Soviet std	MS var	MS var	Other
			ug/l		ug/l		ug/l		ug/l	ug/l	ug/l	ug/l	
218019 99587	chrysene	C18H12	x										
7	cresol-a-, p-chlere-	C7H7ClO	x										
6	cresol-a-, 6-chlere-	C7H7ClO											
1321104	cresol, chlere-	C7H7ClO											
534521	cresol, 4,6-dilatre-	C7H6Cl2O5	x										
21	crotonitrile	C4H5N											
99828	cumene	C9H12											
110827	cyclohexane	C6H12											
37	cyclohexane, nitro-	C6H5NO2											
100930	cyclohexanol	C6H12O											
160544	cyclohexane oxide	C6H11O											
117938	cyclohexene	C6H10											
77474	cycloheptadiene, benzochlere-	C8H16	x										
621647	di- <i>a</i> -propyltetracaine	C6H14Cl2O2	x										
132649	diisobutylbenzene	C12H20											
53703	diisobutyl phenylacetate	C22H14	x										
77587	ditynol tin dilaurate	C32H40O5S											
34	dichloroetheridrio	C3H6Cl2											
31	diethyl ether maleate	C16H32O											
32	diethyl tin dicaprylate	C4H11N											
109997	diethylamine	C4H11N											
53185	diethylamine, <i>N</i> -nitroso-	C4H10N2O											
111456	diethyline glycol	C4H10O3											
100189	disopropylamine	C6H15N											
33	distethyl phenyl carboxyl	C9H12O											
124403	distylylamine	C2H7N											
82759	distylyl tetracaine	C26_20	x										
25136554	diethane, chloro-	C6H12O2											
1746016	diethane, dimethyl-	C12H4C14O2	x										
75336	diethoxyethane, 1,1-dichlere-	C2H4Cl2	x										
71556	diethoxyethane, 1,1,1-trichlere-	C2H3Cl3	x										
79005	ethane, 1,1,2-trichlere-	C2H3Cl3	x										
79345	ethane, 1,1,2,2-tetrachlere-	C2H2Cl4	x										
107062	ethane, 1,2-dichlere-	C2H4Cl2	x										
75014	ethene, chloro-(viny) chloride	C2H3Cl	x										
127184	ethene, tetrachlere-	C2Cl4	x										

Table A-1. (Continued).

CSIS#	Substance	Formula	EPA pp	EPA advise*	NAS series	NAS std	Soviet std	WGS test	Other
mg/l									
79016	ethene, trichloro-	C2HCl3	x	1d/2.	1d/0.105	0.03			car
75354	ethene, 1,1-dichloro-	C2H2Cl2	x	1d/0.2	7d/0.015	c/0.075			car
540590	ethene, 1,1-dichloro- (trans)	C2H2Cl2	x	1d/1.0		c/0.07			car
542881	ether, bis(chloromethyl)-	C2H4Cl20	x	1d/2.7					
111444	ether, bis(2-chloroethyl)-	C4H8Cl20	x						
106601	ether, bis(2-chloroisopropyl)-	C6H12C120	x						
101553	ether, 4-bromophenoxy phenyl-	C12H12BrO	x						
7005723	ether, 4-chlorophenoxy phenyl-	C12H12ClO	x						
107211	ethylene glycol	C2H6O2							
206440	fluoranthene	C16H10	x						
86737	fluorene	C13H10	x						
50000	formaldehyde	CH20		1d/0.03					
68247961	fuel oil #2	C7H7		1d/0.1					
				1d/0.1					
110029	furan	C4H6O							
543497	heptan-2-one	C7H16O							
111706	heptyl alcohol	C7H16O							
319868	hexachlorocyclohexane, delta-	C6H4Cl6	x						
319846	hexachlorocyclohexane, alpha-	C6H4Cl6	x						
319857	hexachlorocyclohexane, beta-	C6H4Cl6	x						
70304	hexachloroethane	C13H6Cl6O2	x						
124094	hexamethylene diamine	C6H16N2							
100970	hexamethylene tetramine	C6H12N4							
519786	hexan-2-one	C7H14O							
25054705	hexanate	C10H6Cl16O3							
110543	hexane	C6H14							
302012	hydrazine	N4H2							
100630	hydrazine, phenyl-	C6H6N2							
122667	hydrazine, 1,2-diisopropyl-	C12H12N2	x						
193395	Indeno[1,2,3-cd]pyrene	C22H12	x						
35	isocrotonitrile	C4H5N	x						
78591	isophorone	C9H14O	x						
75310	isopropylamine	C3H9N							
143500	ketone	C10C11O							
8003206	kerosene	C10-C16 HCS		1d/0.1					
				1d/0.1					

Table A-1. (Continued).

CAS#	Substance	Formula	EPA #	EPA advis. ^a	NAS #	NAS advis. ^a	MSD std	MSD std	Sorlut std	MSD car	MSD car	Other
mg/l												
75065	lactoacrylate, 2-methyl-	CC(=O)C(C)C(=O)O					0.001	0.0001	0.0001			
107277	mercury, chloroethyl-	CCl ₂ HgCl					0.0001	0.0001	0.0001			
627441	methacrylic acid, methyl ester	CC(=O)C(C)C(=O)O										
60526	methane, bis(2-(chloroethyl))-	CSN(C)C(C)C(C)S										
111191	methane, bromo-	CCBr	x									
74839	methane, bromochloro-	CCBrCl	x									
75274	methane, bromochloro-	CCBrCl	x									
74873	methane, chloro-	CCCl	x									
124481	methane, chloromethyl-	CCBrCl	x									
75092	methane, dichloro-	CC ₂ Cl ₂	x									
75718	methane, dichlorofluoro-	CC ₂ F ₂	x									
56235	methane, tetrachloro-	CC ₄	x									
75252	methane, tribromo-	CCBr ₂	x									
67663	methane, trichloro-	CCBrCl ₂	x									
75694	methane, trichlorofluoro-	CC ₂ FBr	x									
74895	methylanilic acid	CN(S)(=O)c1ccccc1										
90153	octa(h-1-1)	C ₁₀ H ₁₆ O										
135193	octa(h-2-0-1)	C ₁₀ H ₁₆ O										
91203	octahydronaphthalene	C ₁₀ H ₁₆	x									
135891	octahydronaphthalene, hexachloro-	C ₁₀ H ₁₂ Cl ₆										
222131	octahydronaphthalene, octachloro-	C ₁₀ H ₁₂ Cl ₈										
1321646	octahydronaphthalene, pentachloro-	C ₁₀ H ₁₂ Cl ₅										
42	octahydronaphthalene, trichloro-	C ₁₀ H ₁₂ Cl ₃										
1321659	octahydronaphthalene, 2-chloro-	C ₁₀ H ₁₂ Cl										
91537	octahydronaphthalene, 2-methyl-	C ₁₁ H ₁₀										
117706	octa(h-1,4-phenylene, 2,3-dichloro)	C ₁₀ H ₈ Cl ₂										
922613	nitroso(4-h-tertbutylaniline)	C ₁₀ H ₁₀ N ₂ O ₂										
143004	oxygenated alcohols	C _n H _{2n} O										
769205	p-dioxane	C ₄ H ₈ O ₂										
105113	p-dioxane	C ₄ H ₈ O ₂										
123911	p-dioxane	C ₄ H ₈ O ₂										
1103653	p-phenoxyendosulfite	C ₁₀ H ₁₂ O ₄ S ₂										
1107691	pbc (acrolein 1254)	C ₁₂ H ₁₅ Cl ₅ (7)	x									
1110422	pbc (acrolein 1221)	C ₁₂ H ₁₅ Cl ₃ (7)	x									
1114115	pcb (acrolein 1232)	C ₁₂ H ₁₅ Cl ₃ (7)	x									
53469219	pcb (acrolein 1242)	C ₁₂ H ₁₅ Cl ₃ (7)	x									
12672236	pcb (acrolein 1260)	C ₁₂ H ₁₅ Cl ₄ (7)	x									
11026825	pbs (acrolein 1200)	C ₁₂ H ₁₅ Cl ₆ (7)	x									

Table A-1. (Continued).

CAS#	Substance	Formula	EPA pp	EPA advise	NAS start*	NAS act†	NAS std	Steric 314	WPS tex	Other
mg/l										
136254	pentane	C11H12C1503								
850108	phenanthrene	C14H10	x							
108952	pheno l	C6H6O	x							
108430	pheno l, 2-chloro-	C6H5ClO								
554047	pheno l, 2-nitro-	C6H5NO3								
100027	pheno l, 3-nitro-	C6H5NO3								
87865	pheno l, pentachloro-	C6AC150	x							
95578	pheno l, 2-chloro-	C6H5ClO	x							
95607	pheno l, 2-methyl-	C7H8O								
88755	pheno l, 2-nitro-	C6H5NO3	x							
4	pheno l, 2,3-dichloro-	C6AC120								
58902	pheno l, 2,3,4,6-tetrachloro-	C6AC2C140								
120832	pheno l, 2,4-dichloro-	C6H5Cl120	x							
105679	pheno l, 2,4-dimethyl-	C6H10O	x							
51285	pheno l, 2,4-dinitro-	C6H4N2O5	x							
95954	pheno l, 2,4,5-trichloro-	C6H3C130								
88052	pheno l, 2,4,6-trichloro-	C6H3C130	x							
3	pheno l, 2,5-dichloro-	C6H5Cl120								
87656	pheno l, 2,6-dichloro-	C6H5Cl120								
2	pheno l, 3,4-dichloro-	C6H4C120								
105469	pheno l, 4-chloro-	C6H5Cl10								
117817	phthalate, bis (2-ethylhexyl),	C24H42O4	x							
85607	phthalate, butyl benzyl	C18H20O4	x							
84762	phthalate, 61-a-betyl	C19H21O4	x							
11780	phthalate, 61-a-octyl	C24H42O4	x							
89442	phthalate, diethyl	C12H14O4	x							
131113	phthalate, dimethyl	C10H10O4	x							
109068	piceol-2-one	C6H7N								
88691	picric acid	C6H3N3O7								
133633	polychlorinated biphenyls	C12H7Cl7	x							
25267156	polychloroprene	C10H10C18								
40	propane, chlorotrifluoro-	C3H4ClF3								
106936	propane, 1-chloro-2,3-epoxy-	C3H5ClO								
78075	propane, 1,2-dichloro-	C3H5Cl2								
542756	propane, 1,3-dichloro-	C3H4Cl2	x							

Table A-1. (Continued).

CAS#	Substance	Formula	EPA pp	EPA advis*	NAS serv†	NAS ad‡	WHO std	Soviet std	WPS tox	Other
mg/l										
129000	pyrene	C ₁₆ H ₁₀	x							
110861	pyridine	C ₅ H ₅ N								0.2
17	pyridine, 2,5-diethyl-	C ₇ H ₉ N								0.05
120809	pyrocatechol	C ₆ H ₄ O ₂								
121824	pyrox (hexogen or cyclonite)	C ₆ H ₂ O ₆								10/2.2
168463	resorcinol	C ₆ H ₃ O ₂								0.1
39	sodium adipate	C ₆ H ₁₀ O ₄ ·2H ₂ O								
633181	stannane, dibutyltinchloro-	C ₁₁ H ₁₆ O ₂ Sn								1.
597648	stannane, tetraethyl-	C ₂₂ H ₅₀ Sn								0.002
100425	styrene	C ₈ H ₈								0.0002
108863	toluene	C ₇ H ₈	x							
99990	toluene, p-nitro-	C ₇ H ₇ O ₂								
121142	toluene, 2,4-dinitro-	C ₇ H ₅ O ₄	x							
606282	toluene, 2,6-dinitro-	C ₇ H ₅ O ₄	x							
5103719	trans-chloro- triethylamine	C ₁₀ H ₁₆ ClN ₃	x							
121448	xylylene	C ₈ H ₁₆								
1330207		C ₁₀ H ₁₀								
95476	e-xylene	C ₁₀ H ₁₀								

*Duration is shown as number of days (d) or as chronic (c).

- EPA pp = Environmental Protection Agency, priority pollutant
- EPA advis = EPA health advisory
- NAS serv† = National Academy of Sciences, safe no adverse response level
- NAS ad‡ = National Academy of Sciences, acceptable daily intake
- WHO std = World Health Organization standards
- Russian standards
- WPS tox = water quality standards for toxicity (EPA)
- car = carcinogen
- haz = hazardous compound not designated as a priority pollutant

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APPENDIX B**LETHAL DOSES USED IN THE CALCULATION
OF SCREENING CONCENTRATIONS FOR TOXICITY**

The screening concentrations for toxicity are calculated as the product of an oral LD₅₀ for a mammalian species (median lethal dose to 50% of a population of laboratory animals), a risk factor for establishing a threshold concentration for systemic toxicity in humans, body weight of the average soldier, and drinking-water consumption (see section entitled "Screening Concentrations for Toxic and Organoleptic Responses" for a discussion of this procedure). The LD₅₀ data in Table B-1 were obtained from a computer tape of the Registry of Toxic Effects of Chemical Substances (RTECS).¹ For each substance we selected the lowest oral LD₅₀ for a mammalian species. If an oral LD₅₀ was unavailable, we used an LD₅₀ resulting from an intraperitoneal administration. If neither oral nor intraperitoneal doses were available, we used the lethal dose low (LDLo), which is defined as "the lowest dose (other than LD₅₀) of a substance introduced by any route, other than inhalation, over any given period of time in one or more divided portions and reported to have caused death in humans or animals."¹ We restricted our use of the LDLo to those resulting from oral doses to animals. Table B-1 also contains the cited reference in the CODEN abbreviation form reported in the RTECS. All of the CODEN abbreviations are found in Vol. 2 of the 1980 RTECS report.² In Table B-2 we have defined the various acronyms for species and exposure mode used in Table B-1.

Table B-1. Oral LD₅₀'s for organic water contaminants. Each LD₅₀ is for the most sensitive mammalian species.

Table B-1. (Continued).

Table B-1. (Continued).

CASID	SUBSTANCE	LETHAL DOSE*	ROUTE SPECIES	ORIGINAL REFERENCE**
206440	FLUORANTHRENE			
500000	FORMALDEHYDE			
1100999971	FURAN	TETRAHYDRO-		
1100999971	HEPTAN-2-OL			
1100999971	HEPTYL ALCOHOL			
1100999971	HEXACHLOROPHENE			
1100999971	HEXAETHYLENEDIAMINE			
1100999971	HEXANAL			
1100999971	HEXANOL-1			
1100999971	HEXANOL-2			
1100999971	HYDRAZINE			
1100999971	1,2-DIPHENYL-			
1100999971	HYDRAZINE. PHENYL-			
1100999971	IMID-2-AZOBIDIMETHIONE			
1100999971	ISOPROPYLAMINE			
2500000000	KEROSENE			
2500000000	LACTONITRILE.	2-METHYL-		
2500000000	LIMONENE	CHLOROETHYL-		
2500000000	MERCURY CHLORIDE	ACID. METHYL ESTER		
2500000000	METHACRYLIC ACID	(2-CHLOROXY)-		
2500000000	METHACRYLIC ACID, METHYL			
2500000000	METHANE	BIS(2-CHLORO-		
2500000000	METHANE	CHLORO-		
2500000000	METHANE	BROMODICHLORO-		
2500000000	METHANE	BROMOTRICHLORO-		
2500000000	METHANE	DIBROMOCHLORO-		
2500000000	METHANE	DICHLORO-		
2500000000	METHANE	DIODO-		
2500000000	METHANE	TRIACHLORO-		
2500000000	METHANE	TRICHLORO-		
2500000000	METHANE	TRICHLOROFLUORO-		
2500000000	METHANE	TRICHLORONITRO-		
2500000000	METHANE	N,N-DIMETHYLACETATE		
2500000000	METHANE	NAPHTH-1-O		
2500000000	METHANE	NAPHTH-2-O		
2500000000	METHANE	NAPHTHALENE		
2500000000	METHANE	1,2,3,4-TETRAHYDRO-		
2500000000	METHANE	1,2,3,4-TETRAHYDRO-		
2500000000	METHANE	1,2-CHLORO-		
2500000000	METHANE	2-METHYL-		
2500000000	METHANE	2-HEXACHLORO-		
2500000000	METHANE	2,3-DICHLORO-		
2500000000	METHANE	2,3-QUINONE.		
2500000000	METHANE	2,3-QUINONE DIOXIME		
2500000000	METHANE	P-DIOXANE		
2500000000	METHANE	P-PHENYLENEDIAMINE		

Table B-1. (Continued).

Table B-1. (Continued).

CASID	SUBSTANCE	LETHAL DOSE*	MODE SPECIES	ORIGINAL REFERENCE**
606202	TOLUENE, 2,6-DINITRO-	1.77E+02	ORL	MTIS** PB214-270
99081	TOLUENE, M-NITRO-P-NITRO-	3.30E+02	ORL	CHABAS 73-910;5E,70
99990	TOLUENE, P-NITRO-	3.1E+03	ORL	MTIS** PB214-270
121448	TRIETHYLAMINE	4.69E+02	ORL	AMIHAB 4-19-51
5064313	TRISODIUM NITRILOTRIACETATE	4.81E+02*	ORL	NCIILB* NIH-NCI-E-C-72-3252
571346	UREA	5.11E+02*	ORL	AJPHAP 153(1)41-48
121346	VANILLIC ACID	5.02E+03	TPR	COREAF 243 609 56
1330207	XYLENE	4.30E+03	ORL	AMIHAB 14-387-56

* LDLo.

** Original reference CODEN from Registry of Toxic Effects of Chemical Substances (RTECS).²

Note: For each substance we selected the lowest LD₅₀ for a mammalian species. If an oral LD₅₀ was unavailable, we used an LD₅₀ resulting from an intraperitoneal administration. If neither oral nor intraperitoneal doses were reported, we used the lethal dose low (LDLo).

Table B-2. Abbreviations used in Table B-1 for exposure mode and species.

Abbreviations	Definition
ORL	Oral administration
IPR	Intraperitoneal administration
RBT	Rabbit
MUS	Mouse
GPG	Guinea pig
DOM	Domestic animal
CTL	Cattle
MAM	Mammalian species

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APPENDIX C**TASTE AND ODOR THRESHOLDS**

Table C-1 contains the taste- and odor-threshold data that we acquired on organic substances that are potential contaminants in field-water supplies. The data were gathered from a number of different sources, and consequently the threshold values between substances are not strictly comparable because of different methods for determining thresholds. Another artifact of the taste/odor studies is the statistic used for reporting the organoleptic data. In some studies a minimum value is reported; in others an average value. Under the column entitled "TYPE" we have designated whether the concentrations were a minimum (M) or average (A); taste (T) or odor (O) value, based on our review of the reference. Some threshold concentrations in water were calculated from odor thresholds in air using Henry's law constant; these calculated values are identified by a "C" in the column entitled "TYPE."

Table C-1. Reported taste- and odor-detection threshold concentrations (mg/L) for organic chemicals for which we compiled water-quality monitoring data.

Table C-1. (Continued)

CASID	SUBSTANCE	TASTE/ODOR THRESHOLD	TYPE*	REFERENCE**
6	CRESOL-O, 4-CHLORO-	1.80E+00	OM	EPA80S
98828	CUMENE	8.00E-04	DAC	AM0083
110827	CYCLOHEXANE	1.10E-01	OM	VANG77
108930	CYCLOHEXANOL	1.00E-01	OM	VANG77
77474	CYCLOPENTADIENE, HEXACHLORO-	1.00E-01	OM	LILL78
109897	DIETHYLAMINE	1.70E-01	DAC	AM0083
108189	DIISOPROPYLAMINE	4.70E-01	DAC	AM0083
124403	DIMETHYLAMINE	2.90E-01	OM	VANG77
79345	ETHANE, 1,1,2,2-TETRACHLORO-	1.90E-01	DAC	AM0083
107063	ETHANE, 1,2-DICHLORO-	1.90E-01	OM	VANG77
75003	ETHANE, CHLORO-	1.90E-01	DAC	AM0083
67721	ETHANE, HEXACHLORO-	1.00E-01	OM	FAZZ78
64175	ETHANOL	1.00E-01	DAC	AM0083
		1.00E-01	OM	VANG77
		1.00E-01	OM	VANG77
75354	ETHENE, 1,1-DICHLORO-	1.40E-01	DAC	AM0083
540590	ETHENE, 1,2-DICHLORO-	1.60E-01	DAC	AM0083
75014	ETHENE, CHLORO-(VINYL CHLORIDE)	1.60E-01	DAC	AM0083
127184	ETHENE, TETRACHLORO-	1.70E-01	DAC	AM0083
79016	ETHENE, TRICHLORO-	1.00E-01	OM	VANG77
111444	ETHER, BIS(2-CHLOROETHYL)	1.00E-01	OM	VANG77
108601	ETHER, BIS(2-CHLOROISOPROPYL)	1.00E-02	DAC	AM0083
		1.00E-01	OM	FAZZ78
50000	FORMALDEHYDE	1.00E-01	OM	VANG77
110009	FURAN	1.00E-01	OM	VANG77
111706	HEPTYL ALCOHOL	1.00E-01	OM	VANG77
75310	ISOPROPYLAMINE	1.00E-01	DAC	AM0083
75092	METHANE, DICHLORO-	1.00E-01	DAC	AM0083
56235	METHANE, TETRACHLORO-	1.00E-01	DAC	AM0083
75252	METHANE, TRIBROMO-	1.00E-01	OM	VANG77
67663	METHANE, TRICHLORO-	1.00E-01	DAC	ZBET80
74895	METHYLAMINE	1.40E-01	DAC	AM0083
135193	NAPHTH-2-OL	1.00E-01	OM	VANG77
91203	NAPHTHALENE	1.00E-01	OM	VANG77
		1.00E-01	DAC	FAZZ78
85018	PHENANTHRENE	1.00E+00	OM	AM0083
		1.00E+00	OM	VANG77

Table C-1. (Continued)

* O = odor, T = taste, M = minimum concentration detectable by individuals with sensitive sensory ability, A = average concentration detectable by individuals with average sensory ability, and C = calculated from odor thresholds in air using Henry's law constant.

**** References appear as CODEN abbreviations; the CODEN abbreviations correspond to those listed alphabetically in the reference section for Appendix C.**

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APPENDIX D

DATA ON THE CONCENTRATIONS OF ORGANIC SOLUTES IN FRESH AND SALT WATERS

The data on the concentrations of organic solutes in natural waters are presented in two tables: Table D-1 contains concentration data for fresh waters, including surface and ground waters, and Table D-2 contains data for salt waters. Each table contains the type of water measured; the statistical value reported; the number of samples, if available; the reference identifier; and the geographic location. The acronyms for the water types are as follows: DW - drinking water, FDW - finished drinking water, SW - surface water, GW - ground water, and SALT - salt water. The complete literature citation for each of the reference identifiers is located in the reference section of this appendix. Two types of quality control were used to ensure that the values reported in the computerized data base were correct. First, we compared the values in the data base with those in the original reference to see if they agreed; second, we statistically analyzed the values in the data base to identify values that were very high or very low. Once these outliers were found, we reviewed the source articles to determine whether the reported concentrations were valid.

Table D-1. Fresh-water concentration data for organic substances other than pesticides

Table D-1: (Continued)

TYPE	AVERAGE	MEDIAN	MAXIMUM	NO. SAHP	REFERENCE	PLACE
SUBSTANCE			CONCENTRATIONS MG/L			
ANILINE, P-CHLOR-	SH					
ANILINE, 2-CHLORO-	SH					
ANTHRACENE	FDX	FDX	FDX	FDX	FDX	FDX
ANTHRACENE, 2-METHYL	SH	SH	SH	SH	SH	SH
ANTHRACHINON, 1,5-CHLOR- ANTHRACHINON, 1-CHLOR-						
ANTHRACHINON, 2-DICHLOR- AROCLOR 1254 BENZ(1,2)FLUORENE						
BENZENE						
BENZENE, 1,2,4-TRICHLORO- BENZENE, 1,2-DICHLORO-						

Table D-1. (Continued)

Table D-1. (Continued)

Table D-1. (Continued)

Table D-1. (Continued)

SUBSTANCE	TYPE	AVERAGE CONCENTRATIONS MG/L	MEDIAN CONCENTRATIONS MG/L	MAXIMUM CONCENTRATIONS MG/L	NO. SAMPLE	REFERENCE	PLACE
CUMARIC ACID (PARA)	FDN SK	1.00E-06					
CRESOLS	SK	1.70E-05					
CYCLOPENTADIENE, HEXACHLORO-	SH	5.00E-05					
DIBENZOFURAN	FDN FDX SK	5.00E-05					
DIBENZOTHIOPHENE	FDN SK	8.50E-05					
DIBENZO[<i>a,h</i>]ANTHRACENE	FDN SK	5.00E-05					
ETHANE, 1,1,1-TRICHLORO-	SH	1.01E-01					
	GH	6.90E-03					
	FDN	2.59E-02					
	FDX						
	SK						
	FDN FDX SK						
	FDN FDX SK						
ETHANE, 1,1:2-TRICHLORO-	SH	3.10E-01					
ETHANE, 1,1-DICHLORO-	FDN FDX SK	7.00E-03					
	FDN FDX SK						
	FDN FDX SK						
ETHANE, 1,2-DICHLORO-	SH	3.10E-01					
	FDN FDX SK						
ETHANE, TRICHLOROTRIFLUORO-	GH	9.62E-02					
ETHANE, 1,1-DICHLORO-	GH	7.32E-02					
ETHANE, 1,2- DICHLORO-	FDN FDX	2.70E-03					

Table D-1. (Continued)

Table D-1. (Continued)

Table D-1. (Continued)

SUBSTANCE	TYPE	AVERAGE	MEDIAN	MAXIMUM	NO. SAMP	REFERENCE	PLACE
		CONCENTRATIONS MG/L					
FDW	FDW	1.50E-05				1 KYES82	DENMARK
FDW	FDW	2.1E-06	0.4	0.5			FINLAND
SM	FDW	2.1E-05					NORWAY
SH	FDW	2.5E-05					JAPAN
SH	FDW	2.5E-05					JAPAN
FDW	FDW	2.5E-05					CANADA
FDW	FDW	2.5E-05					ONTARIO
FDW	FDW	2.5E-05					ONTARIO
FDW	FDW	2.5E-05					ONTARIO
FDW	FDW	2.5E-05					ONTARIO
FDW	FDW	2.5E-05					ONTARIO
FDW	FDW	2.5E-05					ONTARIO
FDW	FDW	2.5E-05					ONTARIO
FDW	FDW	2.5E-05					ONTARIO
SH	FDW	2.5E-05					ONTARIO
SH	FDW	2.5E-05					ONTARIO
SH	FDW	2.5E-05					ONTARIO
SH	FDW	2.5E-05					ONTARIO
SH	FDW	2.5E-05					ONTARIO
SH	FDW	2.5E-05					ONTARIO
FLUORENF.							
HYDROCARBONS INDENO[1,2,3-CD]PYRENE							
ISOBUTANOATE, METHYL, METHANE, BROMOCHLORO- BROMODICHLORO-							

Table D-1. (Continued)

METHANE, BROMOTRICHLORO-
METHANE, DI BROMO-

Table D-1. (Continued)

Table D-1. (Continued)

Table D-1. (Continued)

METHANE: TRICHLOROETHOXY-

MUSK KETONE

MUSK XYLENE

N,N-DIMETHYLANILINE

NAPHTHALENE

Table D-1. (Continued)

Table D-1. (Continued)

Table D-1. (Continued)

Table D-1. (Continued)

SUBSTANCE	TYPE	AVERAGE	MEDIAN	MAXIMUM	NO. SAMP.	REFERENCE	PLACE
				CONCENTRATIONS MG/L			
PHENOL, 2,4,6-TRICHLORO-	SK	5.00E-05	1.20E-04	5.70E-04	HEGM79	NETHERLANDS	
PHENOL, 2,4-DICHLORO-	SK	1.80E-04	1.80E-04	1.80E-04	HEGM79	NETHERLANDS	
PHENOL, 2,5-DICHLORO-	SK	1.60E-04	1.40E-04	2.00E-04	HEGM79	NETHERLANDS	
PHENOL, 2,6-DICHLORO-	SK	1.90E-04	1.80E-05	2.50E-04	HEGM79	NETHERLANDS	
PHENOL, 2-CHLORO-3,4,5-TRICHLORO-	SK	3.00E-05	1.20E-04	2.50E-04	HEGM79	NETHERLANDS	
PHENOL, 3,4-DICHLORO-	SK	1.50E-04	1.50E-04	1.50E-04	HEGM79	NETHERLANDS	
PHENOL, 3,5-DICHLORO-	SK	1.00E-04	1.00E-04	1.00E-04	HEGM79	NETHERLANDS	
PHENOL, 4-CHLORO-	SK	1.90E-03	7.90E-04	1.90E-03	HEGM79	NETHERLANDS	
PHENOL, M-CHLORO-PENTACHLORO-	SK	1.90E-05	3.80E-04	1.90E-05	HEGM79	NETHERLANDS	
PHENOL, 2,4,6-TRICHLORO-	SK	1.90E-04	7.90E-04	1.90E-04	HEGM79	NETHERLANDS	
PHENOL, 3,4-DICHLORO-	SK	1.00E-03	5.50E-04	1.00E-03	HEGM79	NETHERLANDS	
PHENOL, 3,5-DICHLORO-	SK	1.00E-03	3.20E-04	1.00E-03	HEGM79	NETHERLANDS	
PHENOL, 4-CHLORO-	SK	7.30E-04	7.30E-04	7.30E-04	HEGM79	NETHERLANDS	
PHTHALATE, BIS (2-ETHYLHEXYL)	SK	1.20E-02	1.20E-02	1.20E-02	COTR83	UNITED STATES	
PHTHALATE, BUTYLBENZYL	GH	1.70E-01	3.80E-02	1.90E-02	EPAB1	UNITED STATES, NY	
PHTHALIC ACID	GH	1.90E-02	1.90E-03	1.90E-03	MATS77	JAPAN	
PHTHALATE, DI-N-BUTYL	GH	1.00E-03	4.70E-01	1.00E-03	COTR83	UNITED STATES, NY	

Table D-1. (Continued)

Table D-1. (Continued)

Table D-1. (Continued)

**UREA
VANILLIC ACID**

Table D-1. (Continued)

SUBSTANCE	TYPE	AVERAGE	MEDIAN	MAXIMUM	NO. SAMPL	REFERENCE	PLACE
			CONCENTRATIONS MG/L				
XYLENE	SH	1.90E-05	4.40E-04	2.50E-03	321	MATS77	JAPAN
	FDW		3.40E-04	5.90E-04	230	HEST84	UNITED STATES
	FDW		5.90E-04	9.10E-04	186	HEST84	UNITED STATES
	GK	1.00E-03			1	VAND81	NETHERLANDS
	GK	1.00E-01			1	VAND81	NETHERLANDS
	GK	6.00E-01			1	VAND81	NETHERLANDS
	GK	4.00E-01			1	VAND81	NETHERLANDS

Table D-2. Salt-water concentration data for organic substances other than pesticides.

SUBSTANCE	TYPE	AVERAGE CONCENTRATIONS MG/L	MEDIAN CONCENTRATIONS MG/L	MAXIMUM CONCENTRATIONS MG/L	# SAMP	REFERENCE	PLACE
ACETIC ACID							
SALT	SALT	9.40E-06				SCUR75	NE PACIFIC
SALT	SALT	6.41E-06				SCUR75	NE PACIFIC
SALT	SALT	1.03E-05				SCUR75	NE PACIFIC
SALT	SALT	2.23E-06				SCUR75	NE PACIFIC
SALT	SALT	3.00E-06				SCUR75	NE PACIFIC
SALT	SALT	6.00E-06				SCUR75	NE PACIFIC
SALT	SALT	7.50E-06				SCUR75	NE PACIFIC
SALT	SALT	7.70E-06				SCUR75	NE PACIFIC
SALT	SALT	9.50E-06				SCUR75	NE PACIFIC
SALT	SALT	1.40E-05				SCUR75	NE PACIFIC
SALT	SALT	3.56E-05				SCUR75	NE PACIFIC
BENZALDEHYDE					1.03E-05	SAUE81	MEXICO
BENZENE					1.54E-05	SAUE81	GULF OF MEXICO
BENZENE					1.03E-05	SAUE81	GULF OF MEXICO
BENZENE, 1,2-DICHLORO-						SAUE81	MEXICO
BENZENE, ETHYL-						SAUE81	MEXICO
BUTADIENE, HEXACHLORO-						SAUE81	MEXICO
BUTADIENE, THAMES RIVER						SAUE81	MEXICO
						PEAR75	

Table D-2: (Continued)

Table D-2. (Continued)

SUBSTANCE	TYPE	AVERAGE CONCENTRATIONS MG/L	MEDIAN CONCENTRATIONS MG/L	MAXIMUM CONCENTRATIONS MG/L	# SAMP	REFERENCE	PLACE
SALT		1.54E-05					PACIFIC OCEAN
SALT		1.23E-05					PACIFIC OCEAN
SALT		1.95E-05					PACIFIC OCEAN
HEPTANE		4.10E-06					GULF OF MEXICO
HEPTANE		4.40E-06					GULF OF MEXICO
HEPTANE		1.40E-06					GULF OF MEXICO
HEPTANE		1.00E-07					GULF OF MEXICO
HEPTANE		1.20E-06					GULF OF MEXICO
HEPTANE		1.30E-06					GULF OF MEXICO
HEPTANE		1.30E-06					GULF OF MEXICO
HEPTANE		5.10E-06					GULF OF MEXICO
HEPTANE		5.30E-06					GULF OF MEXICO
HEPTANE		2.40E-06					GULF OF MEXICO
HEPTANE		7.50E-06					GULF OF MEXICO
HEPTANE		3.40E-02					GULF OF MEXICO
HEPTANE		1.30E-06					BALTIC SEA
HEPTANE		5.10E-06					BALTIC SEA
HEPTANE		5.30E-06					BALTIC SEA
HEPTANE		2.40E-06					BALTIC SEA
HEPTANE		7.50E-06					BALTIC SEA
HEPTANE		3.40E-02					BALTIC SEA
HEXANAL		5.13E-06					GULF OF MEXICO
HEXANE		2.05E-06					GULF OF MEXICO
HYDROCARBONS							CARIBBEAN SEA
LIMONENE							CARIBBEAN SEA
METHANE		2.05E-06					THAMES RIVER
METHANE		4.35E-05					GULF OF MEXICO
METHANE		6.64E-05					GULF OF MEXICO
METHANE		5.08E-05					GULF OF MEXICO
METHANE		5.94E-05					GULF OF MEXICO
METHANE		4.50E-04					GULF OF MEXICO
METHANE		4.10E-05					GULF OF MEXICO
METHANE, TETRACHLORO-							GULF OF MEXICO
METHANE, TRICHLORO-							GULF OF MEXICO
NAPHTHALENE		2.05E-06					GULF OF MEXICO
NCINANE		3.08E-06					GULF OF MEXICO
NCINANE		2.00E-07					GULF OF MEXICO
NCINANE		2.00E-07					GULF OF MEXICO
NCINANE		2.30E-06					GULF OF MEXICO
NCINANE		1.50E-06					GULF OF MEXICO
NCINANE		9.00E-07					GULF OF MEXICO
O-XYLENE		2.05E-06					GULF OF MEXICO
O-XYLENE		3.08E-06					GULF OF MEXICO
O-XYLENE		2.05E-06					GULF OF MEXICO
O-XYLENE		2.00E-06					GULF OF MEXICO
O-XYLENE		2.60E-06					GULF OF MEXICO
O-XYLENE		3.00E-07					GULF OF MEXICO
O-XYLENE		1.01E-05					GULF OF MEXICO
O-XYLENE		2.30E-06					GULF OF MEXICO
O-XYLENE		1.03E-05					GULF OF MEXICO
O-XYLENE		1.03E-06					GULF OF MEXICO

Table D-2. (Continued)

Table D-2: (Continued)

Table I)-2. (Continued)

Table D-2. (Continued)

SUBSTANCE	TYPE	AVERAGE CONCENTRATIONS MG/L	MAXIMUM CONCENTRATIONS MG/L	# SAMP	REFERENCE	PLACE
SALT		4.10E-06		1	GSCH80	PACIFIC OCEAN
SALT		6.15E-06		1	GSCH80	PACIFIC OCEAN
SALT		6.1.02E-05		1	SAUE78	GULF OF MEXICO
SALT		5.2.20E-05		1	SAUE78	GULF OF MEXICO
SALT		2.1.10E-05		1	SAUE78	GULF OF MEXICO
SALT		2.2.70E-05		1	SAUE78	GULF OF MEXICO
SALT		2.4.4E-05		1	SAUE78	GULF OF MEXICO
SALT		2.9.90E-05		1	SAUE78	GULF OF MEXICO
SALT		9.1.10E-05		1	SAUE78	GULF OF MEXICO
SALT		9.2.22E-05		1	SAUE81	GULF OF MEXICO
SALT		3.5.59E-05		1	SAUE81	GULF OF MEXICO
SALT			3.07E-05	1	SAUE81	GULF OF MEXICO
SALT			7.1.18E-05	1	SAUE81	GULF OF MEXICO
SALT			3.07E-05	3	SAUE81	GULF OF MEXICO

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